ANALYSIS OF POWER GENERATION PROCESSES USING PETCOKE

A Thesis

by

RAMKUMAR JAYAKUMAR

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

MASTER OF SCIENCE

May 2008

Major Subject: Petroleum Engineering

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Chair of Committee,	Maria A. Barrufet
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ABSTRACT

Analysis of Power Generation Processes Using Petcoke. (May 2008)

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Chair of Advisory Committee: Dr. Maria A. Barrufet

Petroleum coke or petcoke, a refinery byproduct, has generally been considered as an unusable byproduct because of its high sulfur content. However energy industries now view petcoke as a potential feedstock for power generation because it has higher carbon content than other hydrocarbons like coal, biomass and sewage residue. This gives petcoke a great edge over other feedstocks to generate power. Models for the two most common processes for power generation, namely combustion and gasification, were developed using Aspen Plus steady state chemical process simulator. Overall plant layouts for both processes were developed by calculating the heat and mass balance of the unit operations. After conducting wide sensitivity analysis, results indicate that one ton of petcoke feedstock can generate up to 4 MW of net available power. Both processes have rates of return greater than 30%, although gasification offers a slightly more attractive opportunity than combustion.

DEDICATION

I dedicate this work to God and to my parents. I am grateful for their support, faith and encouragement which saw me through the program and helped me achieve my goals.

ACKNOWLEDGEMENTS

I would like to thank my committee chair, Dr. Maria Barrufet for her counseling, encouragement, support, and thorough review that resulted in the completion of this research work and report to the industry.

I would like to extend my thanks to Dr. Christine Economides for her support, advice, and review of the work that resulted in the completion of report to the CONACYT.

My special thanks to Dr. Mahmoud El-Halwagi for his willingness to serve on my dissertation committee, and his invaluable suggestions with Aspen simulator, which significantly helped me completing this research work.

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1. INTRODUCTION

1.1 Objective

This study developed simulation models of gasification and combustion systems to analyze the potential to use petroleum coke (petcoke) as feedstock, for energy generation. We also analyzed the compositions of products in both processes; emissions of carbon dioxide (CO_2), nitrogen oxides (NO_x), sulfur oxides (SO_x) and costs including the capital and operating costs. We used Aspen Plus,[1] steady state simulation software, to model the unit operations in the combustion and gasification processes. The study focused on the gasification systems based on the Texaco gasifier. We used, integrated gasification combined cycle (IGCC) and combustion systems based on atmospheric fluidized bed combustion systems (AFBC) for conducting this study. Our study include, a detailed evaluation of gasification and combustion processes, emissions, process performance in terms of net power generated, power required by the unit operations and a general cost analysis including capital and operating expenses.

1.2 Motivation

Rising prices of natural gas observed in recent times have forced energy intensive industries such as glass, cement, and steel to look for alternative sources of industrial

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This thesis follows the style of the *SPE Journal*.

heat and power. In light of current circumstances, petroleum coke (or petcoke) can be considered a very good prospect because of its low cost, high calorific value (in the range of 15,000 Btu/lb), and availability. Although petcoke has a higher heating value than coal, it generally contains a larger percentage of sulfur compounds and heavy metals, leading to corrosion and environmental emission problems that need to be addressed. Petcoke is more difficult to ignite than coal, but start-up schemes can be designed, including petcoke/coal mixtures and recirculation in fluidized bed boiler, that ensure ignition. Once ignited, petcoke is sufficient for the continuous combustion process. Historically, petcoke has been used in cement production and in the iron and steel industry, which account for two-thirds of its use. Another use has been in carbon electrode manufacture. In recent times, it has been looked upon by energy-intensive industries as a potential cost-effective alternative to oil or natural gas for industrial heat and power.[2]

Process industries currently use natural gas for their power requirements. Because the use of natural gas has become a costly option, this project has evaluated the production of power from petcoke by gasification and combustion processes, to use as a substitute for the natural gas. Because petcoke is cheap and has higher heat content than coal, it could be a good alternative to generate power as a substitute for natural gas[3]. Substituting petcoke for conventional resources already in place in process industries appears promising because of recent increases in production of petcoke in the United States. Petcoke can provide heat and power directly; or it can be gasified to produce

syngas, which can then provide heat and power; or it can be combusted to generate power directly. The gasification process captures more of the energy content and is environmentally superior, but it is more capital intensive.

2. LITERATURE REVIEW

This project aimed at developing a simulation model of power generation through combustion and gasification using petcoke normally considered as an industry refuse, as the feedstock. The project focused mainly on the modeling and simulation of petcoke feedstock based on a Texaco gasification process and atmospheric fluidized bed combustion (AFBC) systems. The models used ASPEN Plus modeling software[1], a steady-state process simulation software developed by the Massachusetts Institute of Technology. The main reason to model the integrated gasification combined cycle (IGCC) and atmospheric fluidized bed combustion (AFBC) systems are due to their wide application in the power industry. They have been widely adopted for power production in the industry. The gasification and combustion process are reviewed and explained briefly in this section.

2.1 Petcoke Availability in US

Petcoke is a byproduct of petroleum refineries. Coking feedstocks are generally a result of the heavy crude that cannot be further economically distilled or cracked into lighter components. Petcoke can be produced by delayed coking, fluid coking, and flexi coking. Fig 2.1. shows that the petcoke exports from US have increased steadily over recent years from US refineries. In 1999, US gulf coast refineries contributed 53.40% of US petcoke export quantities (10.36 out of 19.4 MMTPA of total US exports) while the

Californian refineries contributed 28.96% (5.62 out of 19.4 MMTPA of total US exports) of the total export.[3,4]

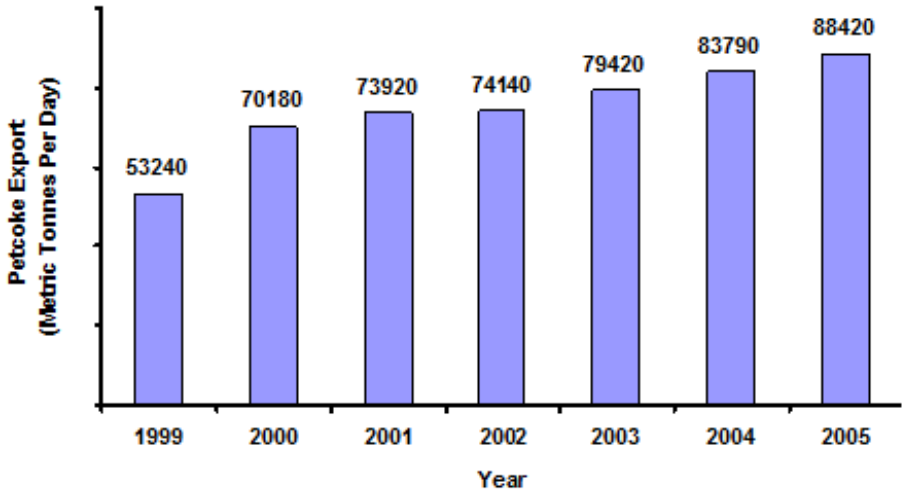

Fig. 2.1 - Petcoke export from US refineries

2.2 Overview of Combustion Systems

Combustion is one of the oldest technologies and the most common method for generating steam. Earlier combustion processes were carried out in fixed beds, then in fluidized beds; the latest technology is at high-pressures. In general, combustion processes around the world use coal, biomass, heavy oil, and refinery wastes as their feedstock for generating steam.

In 2005, US utilities generated 652,312 MW of electricity. Of the total power generated, 62% was generated from combustion turbines, 11% from hydroelectric, 9% from gasification of hydrocarbons, and the remainder from other resources like nuclear power, geothermal, and other renewable energy sources Combined with gasification combustion technology could be seen here as the forerunner in power generation.[5] Fig 2.2 shows the distribution of power generation by each sector in US in the year 2005.

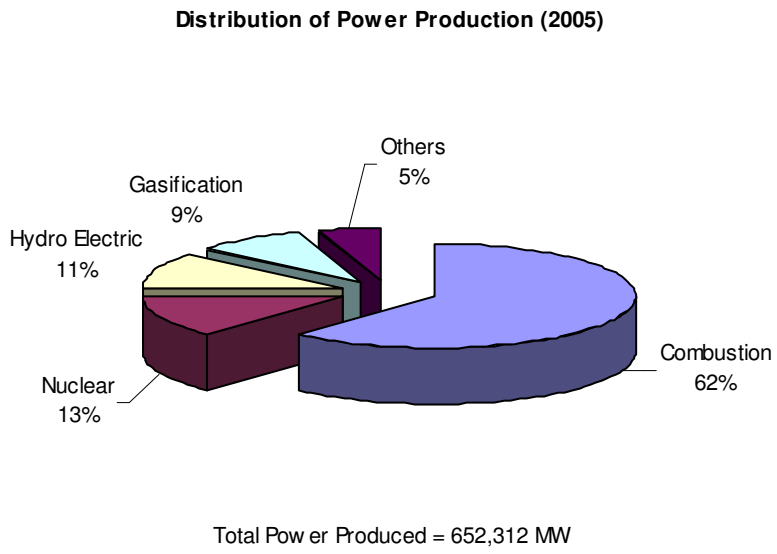

Fig. 2.2 - Distribution of power production in US (2005)

2.3 Combustion Technologies

The two main combustion technologies widely used in the industry are:

1) Atmospheric fluidized bed combustion (AFBC)

2) Pressurized fluidized bed combustion (PFBC).

2.3.1 Atmospheric Fluidized Bed Combustion (AFBC) Process

In the AFBC process, feedstock is dried and ground to a suitable mesh size, usually in the range of 20 to 75 micrometers.[6] It is then fed into the combustor along with excess air, which combusts it completely into products such as carbon dioxide (CO_2) , water vapor (H_2O), nitrogen oxides (NO_x), sulfur oxides (SO_x) and other gaseous combustion products.[7] Heat generated as a result of the combustion is used to generate steam, which is used in the steam turbine to generate power. Fig. 2.3 shows the combustion unit alone in detail.[8] The AFBC combustion unit has a feed inlet that takes in petcoke and limestone. Air enters through the duct at the bottom of the combustor and oxidizes petcoke. Combustion takes place in the combustion chamber where the hydrocarbon is completely burned. Limestone reacts with the sulfur oxides and forms calcium sulfate. Hot flue gas that comes out of the combustor enters the precipitator, which removes ash from the combustion products. Stack gas free of ash exits the combustor and is fed into heat recovery system for steam generation.

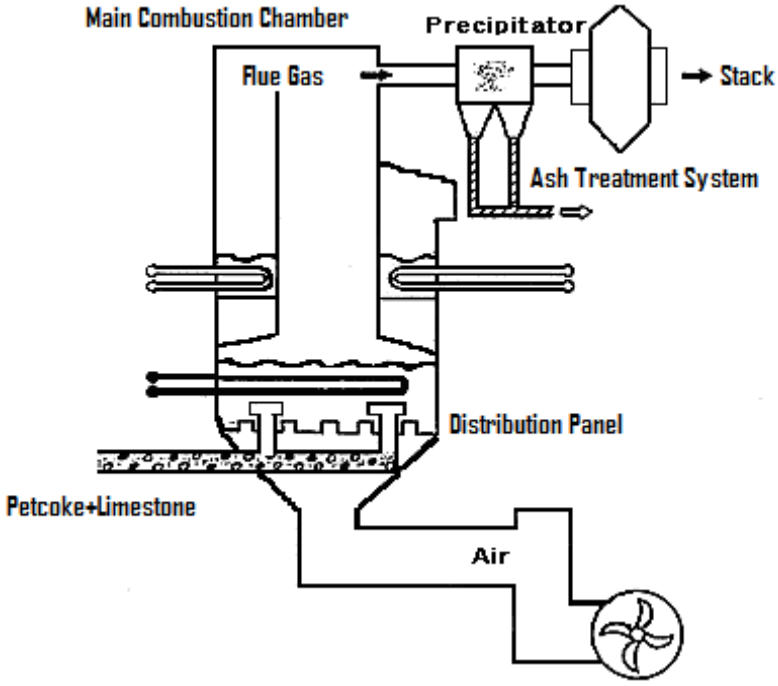

Fig 2.3 - A typical AFBC unit[8]

A typical power generation process using the AFBC Combustion system is shown in Fig. 2.4. It shows the overall flow sheet with typical unit operations such as sulfur removal, heat recovery, NO_x burners used in AFBC plant.

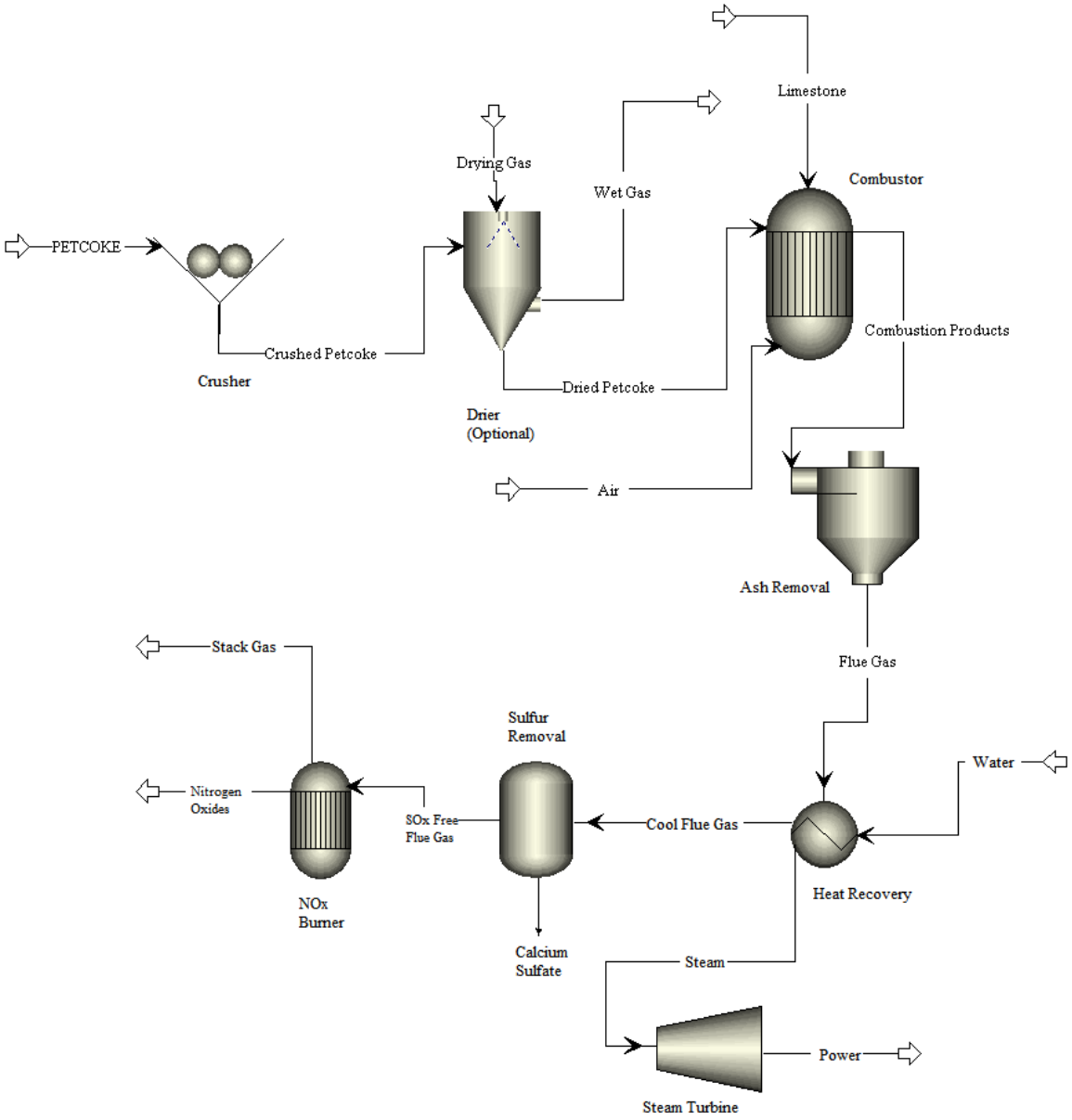

Fig. 2.4 - Typical unit operations flow sheet of the combustion process

2.3.2 Pressurized Fluidized Bed Combustion

A PFBC system operates at an elevated pressure (above 4000 psia).[9] The high-pressure provides gaseous products adequate energy for turbine processes. PFBC

systems generally have higher efficiencies than the AFBC process since they use a combined cycle that consists of gas and steam turbines. Combusted products that come out at elevated pressures are expanded through a gas turbine cycle for additional power generation. The combined cycle ensures power generation during both gas and steam cycles resulting in higher efficiency than that of combined cycle gasification process. Fig 2.5 shows a typical PFBC.[10] In PFBC, petcoke is combusted along with limestone, and the hot flue gas that comes out of the combustor enters the hot gas-cleaning system. Gas cleaning ensures that no sulfur oxides or nitrogen oxides enter the gas turbine section, since the gas turbine is very sensitive to these emission compounds. Since gas requires lower temperatures, the gas is cooled before the products of combustion are fed into the gas turbine. Steam generated during the gas cooling process is redirected to the heat recovery steam generator (HRSG) to be fed into the steam turbine for power generation. Emission control in PFBC is similar to the atmospheric combustion process. Sulfur dioxide is mainly controlled by the addition of limestone or dolomite.

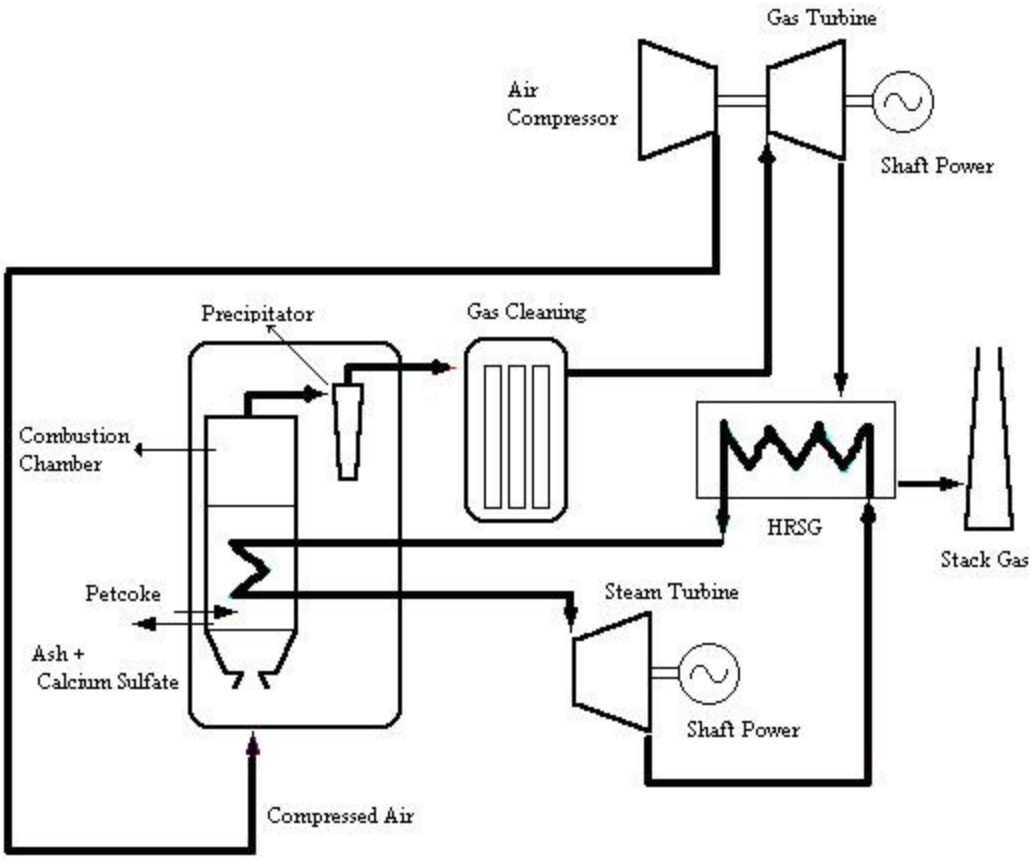

Fig 2.5 - A typical PFBC unit

2.4 Combustion Mechanisms

Combustion involves a series of complex chemical reactions. The general approach is to break down the carbonaceous material into a series of equivalent simple reactions. These reactions take place in a systematic way involving following steps[11]:

1. Devolatilization and volatile combustion
2. Char (C) combustion
3. NO_x formation

4. SO_2 adsorption in limestone, forming calcium sulfate.

2.4.1 Devolatilization and Volatile Combustion

When petcoke is fed into the reactor, it decomposes into two main components: hydrogen-rich volatile fuel and carbon. The moisture content present in the feedstock after drying evaporates during the devolatilization process. Devolatilization and combustion are very fast in AFBC, with mean residence time from 0.4 to 5 seconds.[11, 12] Since the reaction is fast enough to achieve equilibrium at small residence times, we modeled it with equivalent simple reactions involving combustion of elemental components using equilibrium reactors. The steps involved in this modeling of combustion chamber include:

1) Decomposition of petcoke into elemental components
2) Volatile combustion.

Combustion of carbonaceous feedstock always involves complex reactions that are very difficult to model, since the kinetic constants for various series and parallel reactions are unknown. To simplify, the feedstock is decomposed into elemental components based on the ultimate analysis of the feedstock.[11]

Volatile combustion can be written as,

$$\text{Volatiles (HC)} + O_2 \rightarrow CO + H_2O \qquad (1)$$

The main reactions considered in the modeling volatile combustion process are:

- $C + ½\ O_2 \rightarrow CO$ -111 MJ/kmol (2)
- $S + O_2 \rightarrow SO_2$ -296 MJ/kmol (3)

- $H2 + ½\ O_2 \rightarrow H_2O$ -241 MJ/kmol (4)

Exothermic volatile combustion reaction, mainly produce CO and H_2O, and SO_2 release rate is proportional to the char combustion rate.[13]

2.4.2 Char Combustion

Char combustion mainly involves the formation of carbon dioxide and carbon monoxide. The char combustion mechanism proposed by Gordon and Amundson takes into consideration two main reactions.[14] They are:

- $CO + ½\ O_2 \rightarrow CO_2$ -283 MJ/kmol (5)
- $C + CO_2 \rightarrow 2\ CO$ +172 MJ/kmol (6)

The reactions that involve combustion of char (C) are heterogeneous, whereas the carbon dioxide formation reaction takes place in a homogenous phase. The reaction rates depend mainly on physical and chemical properties of char, and in modeling it is considered to take place at equilibrium conditions with fast reaction rates. Temperature is a main criterion for the first four reactions. At temperatures below 350^oF, those reactions are predominant and above the temperature range reactions the last two are predominant.

2.4.3 NOx Formation

During combustion with air, nitrogen present in the fuel or in air reacts with oxygen to form nitric oxide (NO), which reacts further to form nitrogen dioxide (NO_2). In

addition, small amounts of N_2O may be formed during the combustion process.[11, 15] The main reactions involved in the formation of nitrogen oxides are given as:

$$\frac{1}{2} N_2 + \frac{1}{2} O_2 \rightarrow NO \qquad +34 \text{ MJ/kmol} \quad (7)$$

$$\frac{1}{2} N_2 + O_2 \rightarrow NO_2 \qquad -57 \text{ MJ/kmol} \quad (8)$$

$$N_2 + \frac{1}{2} O_2 \rightarrow N_2O \qquad +82 \text{ MJ/kmol} \quad (9)$$

2.4.4 SO_2 Adsorption in Limestone Forming Calcium Sulfate

Limestone is fed into the reactor with coal. At elevated temperatures, limestone decomposes to calcium oxide, which reacts with sulfur dioxide formed during combustion to form calcium sulfate. The reactions are given as:

$$CaCO_3 \rightarrow CaO + CO_2 \qquad (10)$$

$$CaO + SO_2 + \frac{1}{2} O_2 \rightarrow CaSO_4 \qquad (11)$$

Conversion of SO_2 is greatly influenced by the properties of $CaCO_3$, and for simplicity in the modeling a conversion of 99% of SO_2 to $CaSO_4$ is assumed. This assumption is valid if the particle size distribution of $CaCO_3$ is fine in the range of 1 to 50 microns. In our modeling, the $CaCO_3$ particle size distribution is assumed to be same as that of petcoke, modeled within the range of 1 to 50 microns to avoid heterogeneity effects in the reactions 10 and 11.[11]

2.5 Heat Recovery and Power Generation

The products of combustion are normally fed into heat exchangers to recover heat for generating steam. Steam thus generated is run through the steam turbine to generate power. The steam cycle was modeled using a Rankine cycle, as shown in the Fig. 2.6. The cycle begins as the fluid is pumped from a lower pressure (1 on Fig. 2.6) to a higher pressure (2); W_{pump} represents the work expended by the compressors. The fluid is heated by a boiler as shown by the curve from 2 to the isobar at 3. At that isobar, the high-pressure liquid is heated to a saturated-vapor stage. The saturated vapor expands as it follows an isentropic path from 3 to 4. The working fluid condenses along the path 4 to 1, with a heat rejection equivalent to Q_{out}. Process 1 to 2 requires pumping of the fluid from low to higher pressure by the compressors.[16]

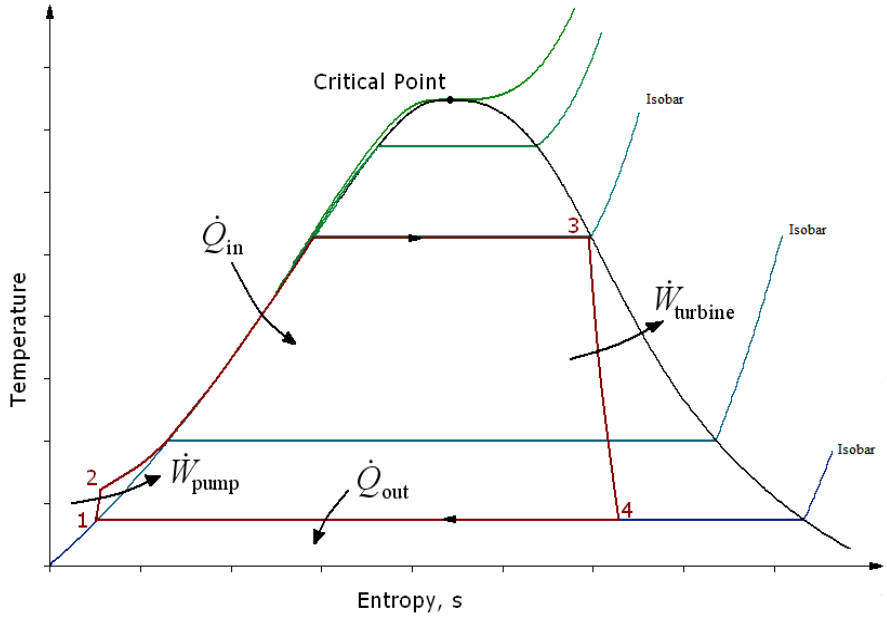

Fig. 2.6 - T-S plot of the Rankine cycle

The main equations used in Rankine cycle are:

$$W_{pump} = \dot{m}(h_2 - h_1) \qquad (12)$$

$$W_{turbine} = \dot{m}(h_3 - h_4) \qquad (13)$$

$$Q_{in} = \dot{m}(h_3 - h_2) \qquad (14)$$

$$Q_{out} = \dot{m}(h_1 - h_4) \qquad (15)$$

where

Q_{in} and Q_{out} represent heat in or heat out of the Rankine cycle,

W_{pump} and $W_{turbine}$ represent work in and work available in the Rankine cycle,

$\dot{m}$ is the mass flow rate of working fluid (steam) in the cycle, and

h_1, h_2, h_3 and h_4 are the enthalpies at specified points in the diagram.

2.6 Overview of Gasification

Recently gasification technology is gaining importance. In gasification, the feedstock is gasified with oxygen to produce product generally called as "syngas", which is a mixture of carbon monoxide (CO) and hydrogen (H_2). In general gasification involves series of chemical reaction of carbon with steam, air or oxygen at temperatures of 1800 ^{o}F to 2800 ^{o}F to produce syngas that can be used to generate power or can be used as raw material for synthesis of chemicals, liquid fuels or gaseous fuels like hydrogen. The oxidizing agent mainly used in gasification is pure oxygen. Sometimes air is also used as an oxidizing agent; in that case, the process is commonly referred to as "air gasification". Steam is generally fed with the feed stream in a gasification process to increase the amount of hydrogen content in the product stream.[2]

2.7 Gasification Systems Around the World

Gasification has gained importance in the industry because it has higher efficiency than the combustion process. As a result of this, there were almost 120 gasification plants in the world by the end of 2004 with total production close to 45,000 MW.[17] Gasification plants with different feedstocks are emerging in countries like China, India, Germany, and Italy. Table 2.1 shows the power capacity of petcoke gasification plants around world.

Table 2.1 Gasification plants around the world with petcoke feedstock[17]

Gasification Technology	Location	Plant Output
GE Gasification	Ube City, Japan	793 MW
E-Gas Gasification	Lima, OH	530 MW
E-Gas Gasification	Terre Haute, IN	262 MW
GE Gasification	Polk, FL	252 MW
Shell Gasification Process	Orissa, India	180 MW
GE Gasification	Delaware City, DE	160 MW
GE Gasification	El Dorado, KS	35 MW

In addition to these, many gasification plants are coming up in US and in other parts of the world. Notable ones in the commissioning process are in Ohio; Corpus Christi (TX); Edwardsport, Indiana; and Taconite, Minnesota. Texaco gasification process is widely used around the world with total production around 20,000 MW. We chose Texaco process for the simulation model because of its wide use around the world.

2.8 Integrated Gasification Combined Cycle (IGCC)

The integrated gasification combined cycle process is a typical gasification technology for converting carbonaceous solid fuels like biomass, coal, and petcoke into synthetic gas (syngas). Its combined power generation technology is unique, with power generation both from gas and steam turbine cycle. A typical integrated gasification combined cycle system is shown in Fig. 2.7.

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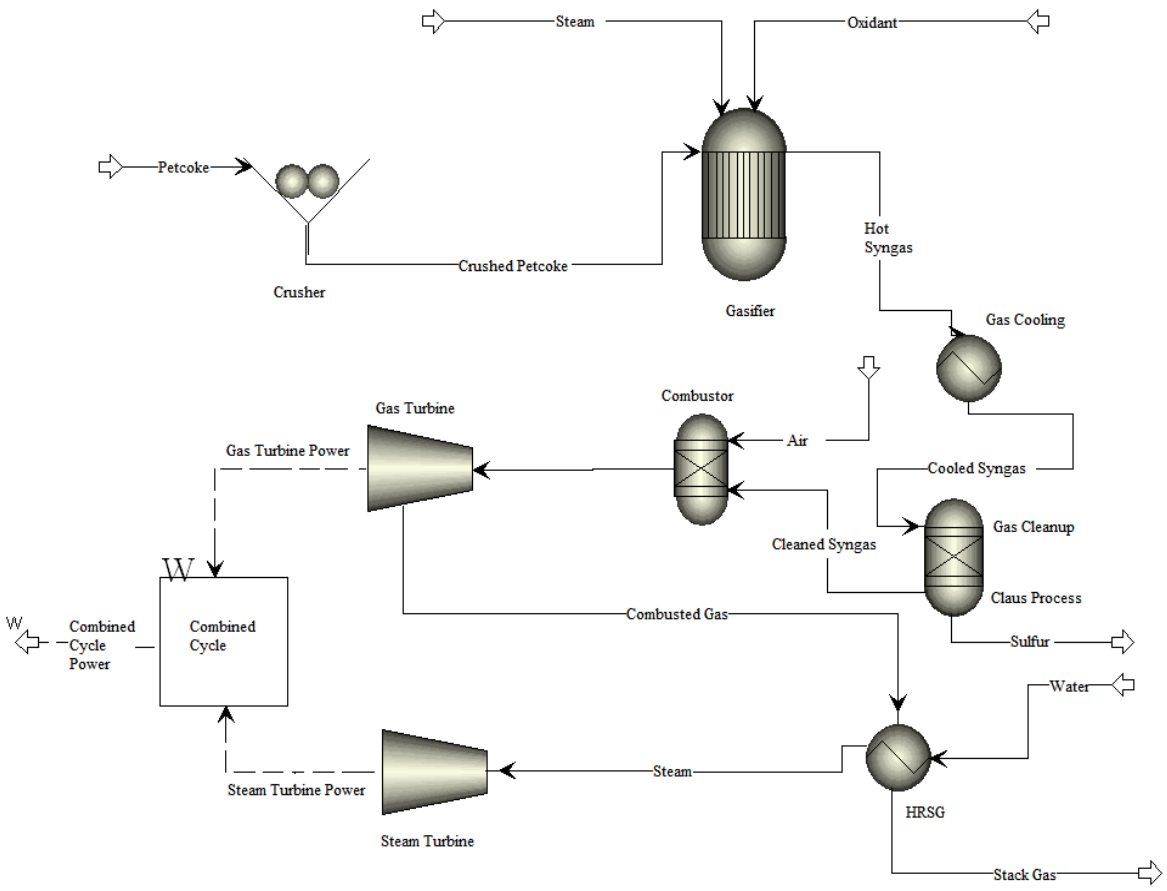

Fig. 2.7 - Typical unit operations flow sheet of the gasification process

2.9 Gasifier Technologies

The three main gasifier technologies used widely are:

1) Fixed bed gasifier
2) Entrained flow gasifier
3) Fluidized bed gasifier

We can see in detail about the three main gasifiers used in the industry.

2.9.1 Fixed Bed Gasification Process

In the fixed bed gasification process (Fig. 2.7), feedstock is loaded through the top into a lock hopper (which is isolated from the reactor during loading), then pressurized and fed into the reactor. The oxidant and steam are fed from the bottom of the reactor. Counter-current flow ensures a good sensible heat usage at low temperatures, (typically in the range of 1,650^{o}F) and also to achieve high carbon conversions (in the range of 99%). But the main drawback of this system is that when large particle size feedstock is used, conversion of the feedstock is much lower than with pulverized feedstock. British Gas Lurgi (BGL) gasifier is a very good example of a fixed bed gasifier. The dimensions of the fixed bed vary from 4 m in diameter and 4 to 5 m in depth. Fig. 2.8 shows a typical fixed bed gasifier. Typical particle size of feedstock for fixed bed gasifier is in the range of 3 to 30 mm. Typical residence time of the moving bed process is around 0.5 to 4 s. [2, 18]

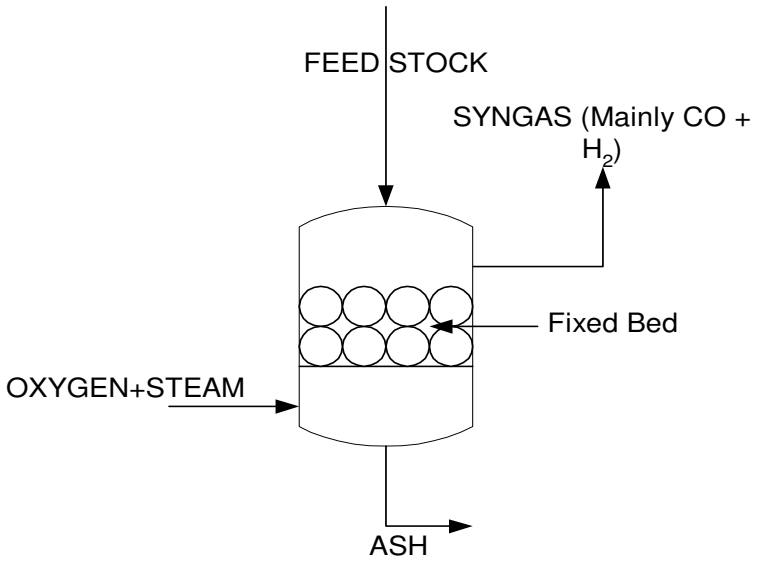

Fig. 2.8 - A typical fixed bed gasifier unit

Fig. 2.9. shows a typical temperature profile of the gas and coal feedstock stream inside a Lurgi moving bed gasifier. In this process, the Boudard and methanation reactions begin before the oxygen is fully consumed. The gases exiting the gasification zone is used to devolatalize and dry the feedstock. Countercurrent flow ensures relatively higher methane content of the outlet gas.

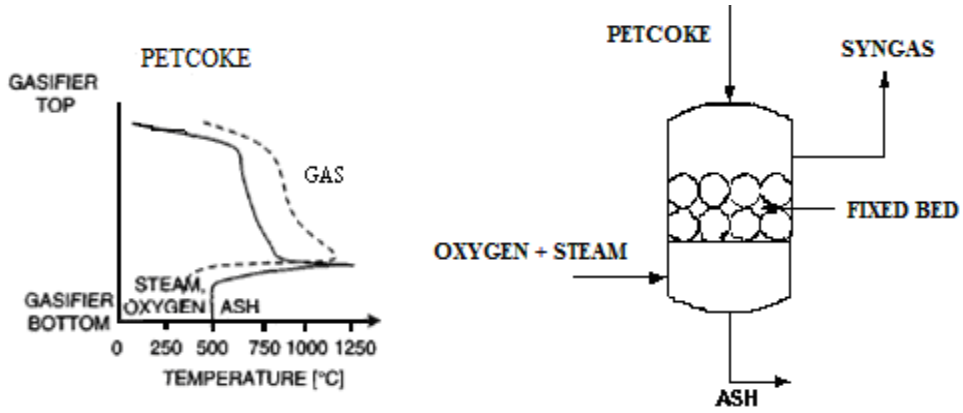

Fig. 2.9 – Temperature profile in a fixed bed gasifier unit[2]

2.9.2 Entrained Flow Gasification Process

In the entrained flow gasification process, feedstock is elutriated by the oxidant and steam stream. The oxidant and steam are fed from the bottom of the reactor, and feedstock is fed through other inlet at bottom of the reactor. The velocity of oxidant and steam stream determines the elutriation of the feedstock particles. For proper elutriation to occur, the feedstock particles must be finely crushed and the oxidant and steam

streams must be fed with high velocity to ensure proper contact between the oxidant and feedstock stream. The Texaco and E-Gas gasifiers use this method for gasifying the hydrocarbon feedstock. Fig. 2.10 shows a typical entrained flow gasifier. Typical particle size of feedstock for entrained flow gasifier is in the range of 0.1 to 0.2 mm. Feedstock size is smaller than the fixed bed process to attain the fluidization in the bed.[2] Typical residence times of the entrained flow process are around 0.5 to 2 s.

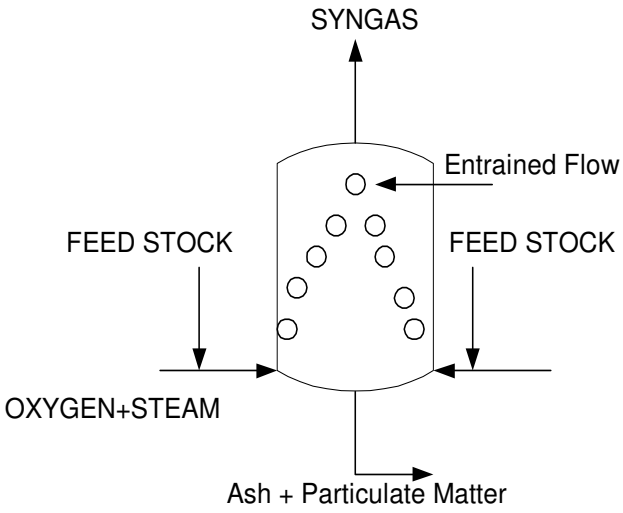

Fig. 2.10 - A typical entrained bed gasifier unit

Fig. 2.11 shows a typical temperature profile of the gas and coal feedstock stream inside a side-fired entrained bed gasifier. The temperature of petcoke increases linearly as the petcoke is consumed through the reactor, as shown in the temperature profile of

the gasifier. This mainly reflects the fact that water vapor is evaporated first, before gasification reactions takes place.[2]

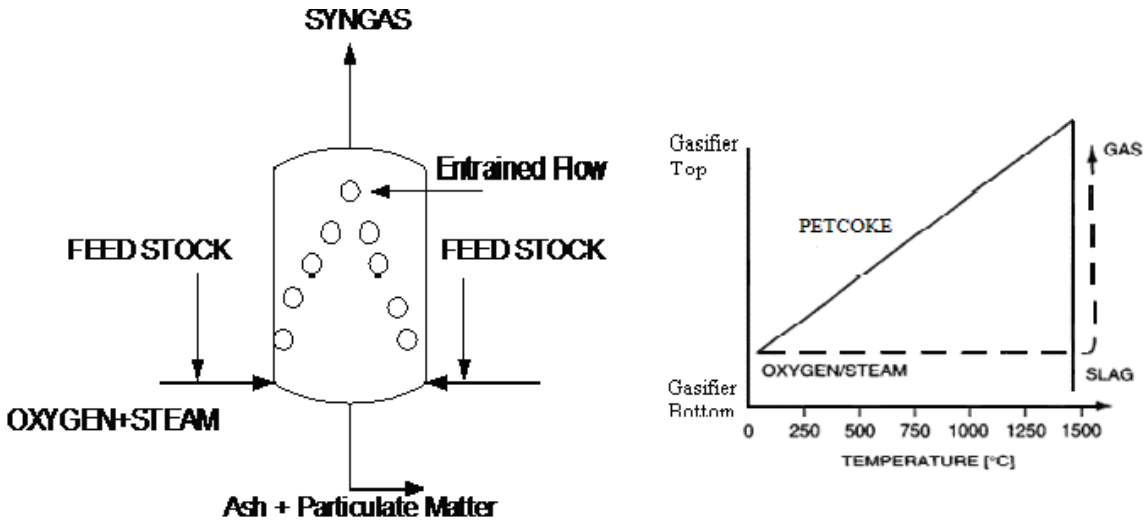

Fig. 2.11 - Temperature profile in a entrained bed gasifier unit[2]

2.9.3 Fluidized Bed Gasification Process

In the fluidized bed gasification process, feedstock is again entrained by the oxidant and steam stream. The oxidant and steam along with the feedstock are fed from the bottom of the reactor, and their velocity determines the fluidization of the feedstock particles. Similar to entrained flow gasifier, feedstock particles are to be finely crushed and also the oxidant and steam streams must be fed with typical high gas velocity of around 5 m/s to ensure proper contact between the oxidant and feedstock stream. Fig.

2.12 shows a typical fluidized bed gasifier. Typical particle size of feedstock for fluidized bed gasifier is in the range of 1 to 5 mm.[2] Typical residence time for fluidized bed are also similar to entrained flow gasifier around 0.5 to 2 s.[19]

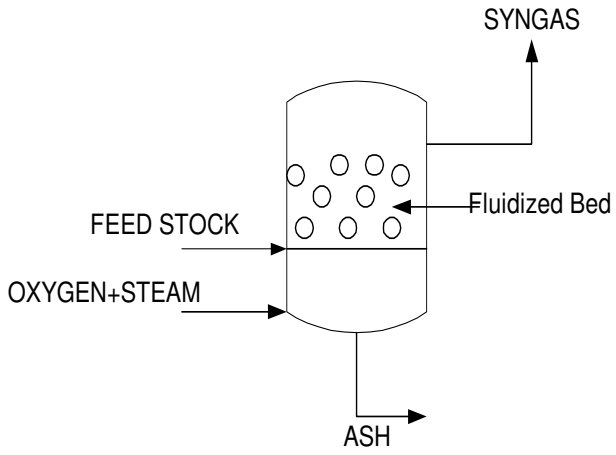

Fig. 2.12 - A typical fluidized bed gasifier unit

Fig. 2.13 shows a typical temperature profile of the gas and petcoke feedstock stream inside a fluidized bed gasifier

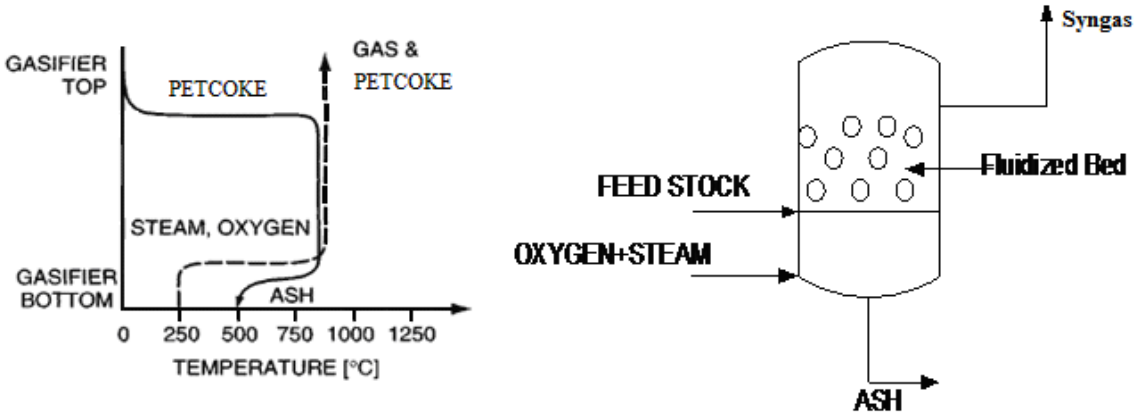

Fig. 2.13 - Temperature profile in a fluidized bed gasifier unit[2]

2.10 Gasification Mechanism

Gasification involves a series of chemical reactions at elevated temperatures and pressures. The temperature is generally maintained around 1,800 to 2,800°F to provide the initial heat for endothermic reactions like the Boudard reaction (Eq. 19) and water gas reaction (Eq. 20). These reactions trigger other main exothermic reactions (Equations 16, 17, 18, 21) to produce CO and H_2. Pressure in a gasifier is usually maintained high to reduce the volume of syngas coming out of the reactor, thereby making the cleanup process much easier. Following are the main reactions which takes place in a gasifier for any hydrocarbon feedstock.[2, 20]

2.10.1 Volatile Combustion reactions

Exothermic combustion reactions are given as:

- $C + ½\ O_2 \rightarrow CO \quad -111$ MJ/kmol (16)

- $CO + ½\ O_2 \rightarrow CO_2$ -283 MJ/kmol (17)
- $H2 + ½\ O_2 \rightarrow H_2O$ -242 MJ/kmol (18)

2.10.2 Boudouard Reaction

The endothermic Boudard reaction is described as,

- $C + CO_2 \rightleftharpoons 2\ CO$ +172 MJ/kmol (19)

with the equilibrium constant given as $K_p = \frac{P^2{}_{CO}}{P_{CO2}} = \frac{(V_{CO})^2}{V_{CO_2}}.P$, where P is the total absolute pressure of the gas. From Boudard reaction we can clearly see that formation of CO is greatly dependent on the pressure. Increase in pressure favors the forward reaction and therefore formation of CO.

2.10.3 Water-Gas Reaction

The water-gas reaction is given as,

- $C + H_2O \rightleftharpoons CO + H_2$ +131 MJ/kmol (20)

with the equilibrium constant given as $K_p = \frac{P_{\ CO} \times P_{H_2}}{P_{H_2O}} = \frac{(V_{CO} \times V_{H_2})}{V_{H_2O}}.P$, where P is the total absolute pressure of the gas. Similarly, reaction 17 is also greatly dependent on the pressure. An increase in pressure favors the forward reaction and favors the formation of CO.

2.10.4 Methanation Reaction

The methanation reaction is given as,

- $C + 2\,H_2 \rightleftharpoons CH_4$ -75 MJ/kmol (21)

In the case of complete conversion of carbon in the feedstock, the Boudouard reaction, the water-gas reaction, and the methanation reaction can be combined into two homogenous reactions namely the CO shift reaction and steam methane reforming reaction.

2.10.5 CO Shift Reaction

The CO shift reaction is given as,

- $CO + H_2O \rightleftharpoons CO_2 + H_2$ -41 MJ/kmol (22)

2.10.6 Steam-Methane Reforming Equation

The steam-methane reaction is given as,

- $CH_4 + H_2O \rightleftharpoons CO + 3\,H_2$ +206 MJ/kmol (23)

These are the main reactions that take place during the solid hydrocarbon gasification process. The equilibrium constant for Eq. 23 is given as:

$$K_p = \frac{P_{CO} \times P^3_{H_2}}{P_{CH_4} \times P_{H_2O}} = \frac{(V_{CO} \times V^3_{H_2})}{V_{CH_4} \times V_{H_2O}}.P$$

Thus, the overall methanation reaction is dependent on pressure. An increase in pressure favors the formation of hydrogen and carbon monoxide greatly. These are the main

reasons to carry out gasification reaction at higher pressures, which favors forward reaction in all the above reactions.

3. MODELING THE COMBUSTION PROCESS

Combustion modeling is explained in this section. The combustion process is divided into six main sections: feedstock preparation, combustion unit, heat recovery unit, power generation unit, sulfur recovery unit, and NO_x control measures.

3.1 Overall Process Flow Description

Fig. 2.5 showed a typical process flow diagram of the combustion process. The petcoke is finely crushed and then fed into the combustor, with limestone and air as oxidant. The usual combustion products are carbon dioxide (CO_2), water (H_2O), sulfur dioxide (SO_2), and nitrogen oxides (NO_x). Combustion products are often referred to as flue gas, which exits the combustor is at a high temperature generally within a range of 1,400 to 2,000^oF.[7] Temperature is selected based on the emission of certain compounds like nitrogen oxides and sulfur oxides. Recent technologies like the pressurized fluidized bed combustion process can provide higher flue gas temperatures, up to 2,200^oF.[7] The heat recovery unit cools the hot flue gas and generates superheated steam for steam turbines in the power generation section. The flue gas then passes through the cleanup system, where the sulfur is removed in the sulfur recovery unit as calcium sulfates, and unburned nitrous oxides are fired in NO_x burners.

3.2 Feedstock

We used the composition of Tuscaloosa petcoke to model the petcoke feedstock in the simulation processes.[22] Tuscaloosa petcoke was chosen for two main reasons.

1. Tuscaloosa petcoke composition generalizes a typical gulf coast petcoke composition.
2. Tuscaloosa petcoke has higher sulfur content of 5.3 wt%. By modeling this process with high sulfur petcoke and curtailing the emissions, we ensured that our model will fit all other best available petcoke with lower sulfur content.

Table 3.1 Proximate analysis of the petcoke feedstock

Components	Weight % (As Received)
Moisture	0.9
Volatile Matter	9.6
Fixed Carbon	88.5
Ash	1.00

Table 3.2 Ultimate analysis of the petcoke feedstock

Components	Weight % (Moisture Free Basis)
Carbon	88.2
Hydrogen	3.8
Nitrogen	1.7
Sulfur	5.3
Oxygen	0.00
Ash	1.00

The proximate and ultimate analysis of the petcoke used in modeling is given in Table 3.1 and Table 3.2. This process is modeled using the stoichiometric reactor in Aspen Plus.

3.3 Feedstock Preparation Unit

The feedstock preparation unit consists of two main unit operations: crushing and drying. Crushing and drying facilitate the easy storage of feedstock in silos for future use. Sometimes two or more various feedstocks are mixed together to get a richer quality of feedstock, which is normally measured in terms of weighted average of the fixed carbon content in the mixture. During such preparation, crushing is the most important unit operation because it maintains the uniformity of the feedstock size to facilitate blending of two different feedstocks.

3.3.1 Crushing

Crushing is a critical feature of the combustion process. The feedstock should be finely ground before being fed into the combustor. Fine particle size increases the burning capacity, facilitates storage and transportation because of its uniform size distribution.

The feedstock is normally stored in a silo and fed into the combustor through a hopper. For the pressurized fluidized combustion process, it is fed through a special hopper called a *lock hopper* that pressurizes the feedstock to up to 250 psia before it is fed into the combustor. The process model assumes that petcoke is crushed to a size range from 1 to 50 microns. The conversion efficiency depends on the particle size; particles in the range of 500 or more microns decrease the conversion of carbon.

3.3.2 Drying

Drying is often an integral part of the feedstock preparation. The drying operation is carried out in an inert atmosphere with nitrogen as the inert medium. Nitrogen is used to remove excess moisture content from the feedstock. Since Tuscaloosa petcoke has only 0.9 wt% of moisture content, the drying process is not included in the process model. Coal, biomass, and other feedstocks may have much higher moisture content (5 to 25 wt%) and would require the drying process.

3.4 Combustion Unit

Combustion is a process of burning fuel such as hydrocarbon feedstock in the presence of excess air or oxygen, converting it to flue gas, which comes out at elevated temperature and produces usable heat. To avoid incomplete combustion and consequent release of carbon monoxide (CO), the normal combustion process is fed with excess air, beyond that required in the stoichiometric reaction. The main flue gas constituents are carbon dioxide (CO_2) and water vapor (H_2O), but contaminants in the hydrocarbon feedstock, principally sulfur, form mainly sulfur dioxide (SO_2) and lesser quantities of sulfur trioxide (SO_3); and nitrogen present in the feedstock forms nitrogen oxides (NO_x).

In the atmospheric fluidized bed combustion (AFBC) process, the small fluidization velocity reduces the amount of feedstock material leaving the reactor, so it is not recycled. The efficiency of AFBC process reported on an average in the literature varies from 25 to 30%.[21, 22]

3.5 Modeling the Feedstock Preparation and Combustion Processes

Feedstock is crushed and dried before it is fed into the combustor. Crushing facilitates the solids handling and improves the efficiency of combustion. If the feedstock is fed into the combustor as lumps, the burning efficiency decreases and thereby increases the amount of un-reacted feedstock coming out of the reactor. Limestone is fed into the reactor along with the feedstock. The crushing unit operation is modeled by the crusher in the flow sheet. If the feedstock has more moisture content in

the range of 10 to 25 wt%, the drying process becomes inevitable. If drying is not employed for wet feedstock, combustion requires more preheat. The important parameters for modeling the crusher are the hardgrove grindability index (HGI) and the bond work index. HGI is a relative grindability measure to define the hardness of the petcoke feedstock with that of coal. The bond work index is a simple measure of minimum percentage of feedstock that should pass through the required mesh size. In our case, a work index value of 80 was used to model the crusher with a mesh size ranging from 1 to 50 microns. The petcoke from the crusher is fed into the decomposition reactor. The decomposition reactor serves to break the non-conventional petcoke feedstock into its constituent elements. The petcoke that comes out of the decomposer flows into the combustor. Air enters the combustor to oxidize the feedstock. The air stream is modeled with a molar ratio of nitrogen to oxygen as 79 to 21. The air stream enters the combustor at a temperature of 77^{o}F and a pressure of 14.7 psia.

Combustion reactions in the combustor are modeled by identifying the possible products. The products that are likely to be formed in a combustion reaction were entered as main parameters for the combustor. The combustion reactions are assumed to take place a temperature of 1,800^{o}F. This temperature was decided after a wide range of sensitivity analysis so as to minimize the emission compounds from the combustor. This assumption is based on the normal temperature range for combustion reaction of 1,400 to 2,200^{o}F[8]. This assumption is valid for conventional combustion reactions, even though nowadays combustion temperatures could go as high as 5,000^{o}F with the use of

special ceramic reactors.[22] By maintaining the lower temperature in the combustor with the help of coolant jacketed system, we generate heat. This heat stream is directed to the secondary heat recovery section, where secondary steam is generated.

The flue gas that comes out of the combustor has ash and some other solid impurities. These are removed by a cyclone separator. Despite its high installation cost, the main advantage of the cyclone over bag filters is that the cyclone can operate at high temperatures. Bag filters are normally limited to a temperature range of 300 to 500^{o}F. The ash-free gas then flows into the calcinizer, which is modeled by a stoichiometric reactor where the calcination reactions are assumed to take place. The reactions are given as:

$$CaCO_3 \longrightarrow CaO + CO_2 \qquad (24)$$

$$CaO + SO_2 + 1/2\ O_2 \longrightarrow CaSO_4 \qquad (25)$$

The limestone stream enters the calcinizer, which is at the exact temperature and pressure conditions of combustor (1,800^{o}F and 14.7 psia). At this high temperature, calcium carbonate breaks down into calcium oxide and carbon dioxide as indicated Eq. 24. Calcium oxide in turn reacts with the sulfur dioxide at this elevated temperature to form calcium sulfate. This is modeled by Eq. 25. The stoichiometric conversions of $CaCO_3$ and CaO in the first and second reactions were assumed to be complete. This assumption is valid since the modern cleanup technologies operate nearly at 100% conversion of sulfur oxides to calcium sulfate.

The ash-free flue gas flows at a temperature of 1,800^{o}F from the calcinizer into the heat recovery section of the process. This is described in the following section. Fig. 3.1 shows the typical flow diagram of the feedstock preparation and combustion process. The main unit operations modeled in the feedstock preparation and combustion section are described in Table 3.3.

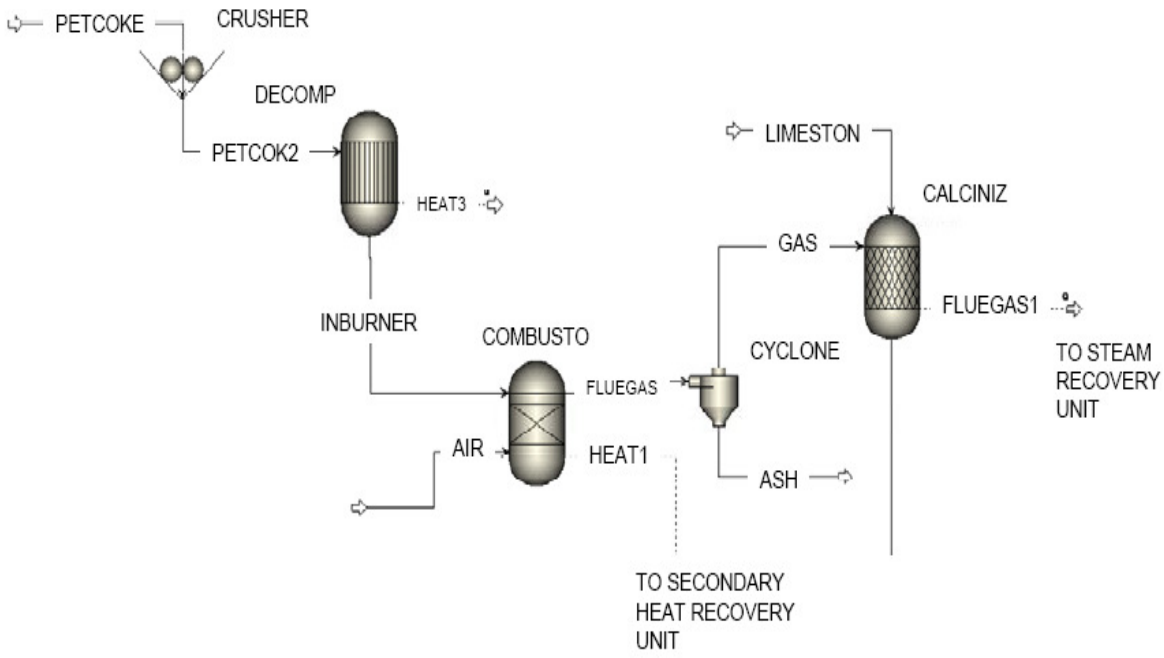

Fig. 3.1 - Flow diagram of combustion section

Table 3.3 Important parameters used for modeling the combustion section

Unit Operation	Modeling Parameters Used
Crusher (CRUSHER)	Maximum Particle Diameter = 50 μm Bond Work index = 80 Hardgrove Grindability Index = 55
Reactor (DECOMP)	Pressure = 14.7 psia Temperature = 77^{o}F
Equilibrium Reactor (COMBUSTO)	Pressure = 14.7 psia Temperature = 1800^{o}F
Separator (CYCLONE)	Efficiency Correlation = Leith-Licht[1] Diameter = 0.5ft
Calcinizing Reactor (CALCINIZ)	Pressure = 14.7 psia Temperature = 1800^{o}F

3.6 Heat Recovery Unit (HRU) and Steam Generation

The heat recovery unit (HRU) is critical to power generation. The HRU model quantifies the amount of superheated steam that can be generated from the flue gas fed from the combustor to the HRU at elevated temperature. Fig. 3.2 shows a general block diagram of an HRU. It consists of three counter-current heat exchangers: the economizer, the evaporator and the superheater. The economizer heats the boiler feed water entering the HRU to its boiling point. In the evaporator section, steam is generated by the change in phase of the saturated water to steam. The latent heat of vaporization is supplied to the boiler feed water by the evaporator. Steam entering the superheater section of the HRU absorbs heat, and the outlet steam temperature is determined mainly by the difference in temperature of the flue gas and the steam outlet temperature. Fig. 3.3 shows the temperature profile of the steam and flue gas in the HRU. [23, 24]

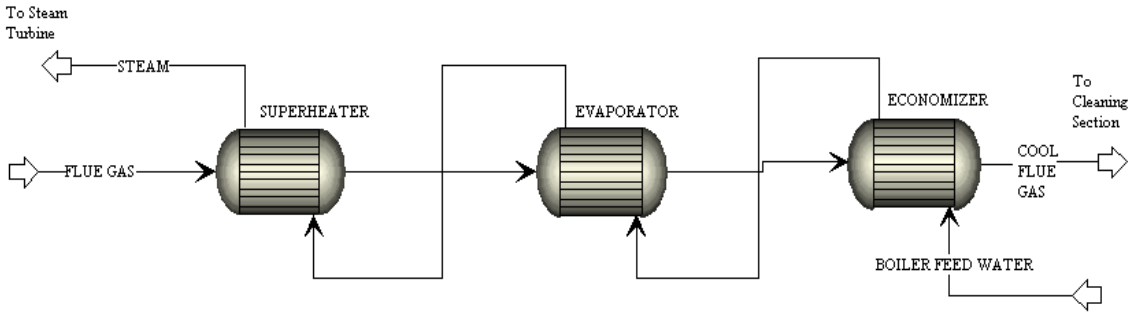

Fig. 3.2 - Flow diagram of heat recovery section

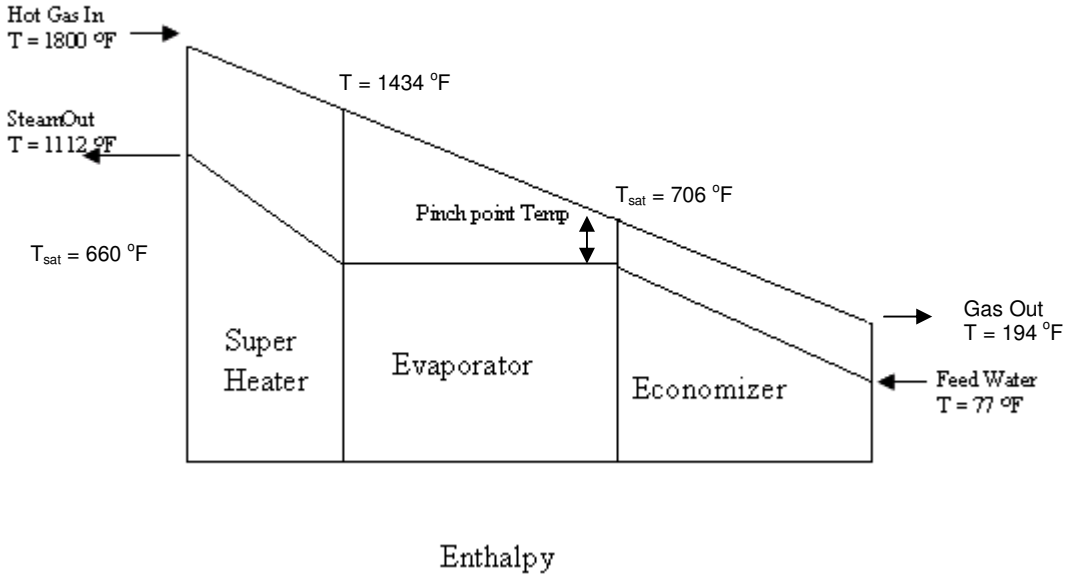

Fig. 3.3 - Pinch point analysis in heat recovery unit

Flue gas leaving the combustion section is at a temperature of 1,800°F enters the steam recovery section. It is modeled by three heat exchangers: the economizer, the evaporator, and the superheater. These heat exchangers are modeled as countercurrent

process. Cooling water enters the economizer, whereas hot flue gas enters the superheater. Coolant is pumped to a pressure of 2,175 psia. The pump is modeled with an isentropic and mechanical efficiency of 0.92. Water at 2,175 psia enters the economizer with a temperature approach of 46^{o}F. Approach temperature was determined by the sensitivity analysis of the economizer. The coolant stream attained vapor fraction at a saturation temperature of 660^{o}F; the heat duty increased above this temperature without any change in the quality of steam.

The saturated coolant stream from the economizer enters the evaporator, which is mainly used for the phase change by supplying latent heat of vaporization. The vapor fraction of the coolant that comes out of the evaporator is modeled to be equal to 1. Coolant then enters the superheater of the heat recovery section. Here the coolant water, which is in the form of saturated vapor, is superheated; the superheat temperature of 1112^{o}F was decided as the temperature of the outlet steam based on the heat duty of the super heater.[24] The flue gas, that enters the superheater, evaporator, and economizer undergoes temperature reduction and comes out of the economizer as cool gas at a temperature of 194^{o}F.

The pinch point is an important part of the power generation process. The steps of our simple algorithmic approach to determine pinch point are:

1. Set arbitrary target values of pressure and flow rate of steam to be generated.

2. Once the arbitrary values are set, construct a flow rate and pressure matrix at which steam has to be generated.
3. Continue the process until we approach the optimum pinch point which maximizes the power generation.

Care should be taken during this analysis. If crossover of temperature is observed in conducting the analysis, it will violate the second law of thermodynamics which states that heat should transfer from hot to a cold substance. Care should also be taken in generating steam from the superheater. Steam generated from the superheater should be in the superheated vapor form for the given pressure and temperature conditions. Obtaining optimum values of pinch point temperature reduces the cost of the heat exchanger. Good pinch point analysis achieves better process integration by maximizing heat recovery and simultaneously reducing the cost of heat exchangers.[8]

Pinch point analysis is an important parameter in determining the total heat available for power generation. The main aim is to transfer the amount of heat as much as possible from the hot stream to the cold stream. In maximizing the heat transfer, care should be taken to avoid the crossover of temperature. Sensitivity analysis was carried out initially by varying two process parameters, the pressure of the outlet steam stream and the flow rate of steam to be generated. During these analyses, we ensured that there is no temperature crossover occurred. The flow rate of the feed water was varied along with various pressure ranges. Table 3.4 shows the sensitivity values with power generated from steam turbines.

Table 3.4 Power generation matrix with feed water flow rate and pressure

Flow Rate (lb/hr)	Pressure (psia)	Flue Gas Outlet Temperature (^oF)	Power Generated from High-pressure Steam Turbine (HP)	Power Generated from Low-pressure Steam Turbine (HP)	Crossover Detected (Y/N)
8578	1600	192.09	3216.28	713.51	N
	1800	192.11	3214.33	711.67	N
	1900	192.13	3216.46	709.88	N
	2000	196.28	3211.65	708.73	N
	2175	203.42	3203.38	706.76	N
	2400	212.32	3193.03	704.30	N
9005	1600	104.21	3269.22	713.51	N
	1800	104.24	3270.64	718.89	N
	1900	103.26	3272.07	720.31	N
	2000	107.57	3267.01	721.74	N
	2175	115.00	3258.33	720.53	N
	2400	124.31	3247.45	718.47	Y
9105	1600	88.45	3301.01	728.28	Y
	1800	88.63	3275.87	722.30	Y
	1900	88.72	3276.38	722.42	Y
	2000	88.81	3276.83	722.53	Y
	2175	88.97	3272.05	721.39	Y
	2400	89.17	3260.67	718.69	Y

From the Table 3.4 we can see that crossover is detected after a certain flow rate and pressure range. Once we identified the optimum values of flow rate and pressure, we set them as the fixed parameters for deciding various other optimum parameters. And other main parameter is the outlet superheat temperature. The superheat temperature was varied from 700^oF to $1,200^oF$. By varying these values, we could analyze the power generated from the steam turbines. Power generation increased with the temperature, as shown in Fig. 3.4. The heat transferred normally to a temperature of $1,118^oF$; once that superheat temperature increased a range crossover was detected. Hence the optimum superheat temperature was found as $1,118^oF$.

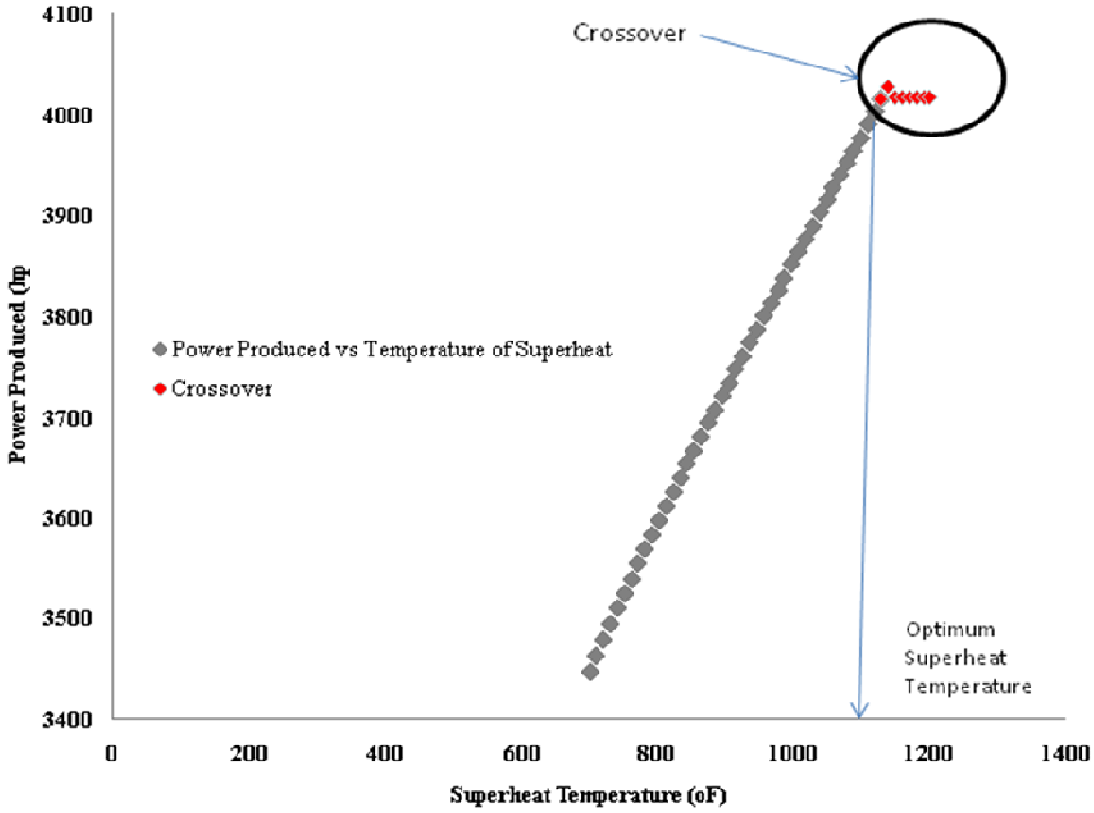

Fig. 3.4 - Power generation variation with temperature

Heat generated from the combustor is used for secondary steam generation. Water is used as the coolant. Water gets heated up and is pumped to a pressure of 2,175 psia. This is done to maintain the same pressure of the steam coming out of the superheater. The steam streams are mixed and fed into the power generation section. Fig. 3.5 and Table 3.5 describe the flow diagram and unit operations used in the heat recovery section of the flow sheet.

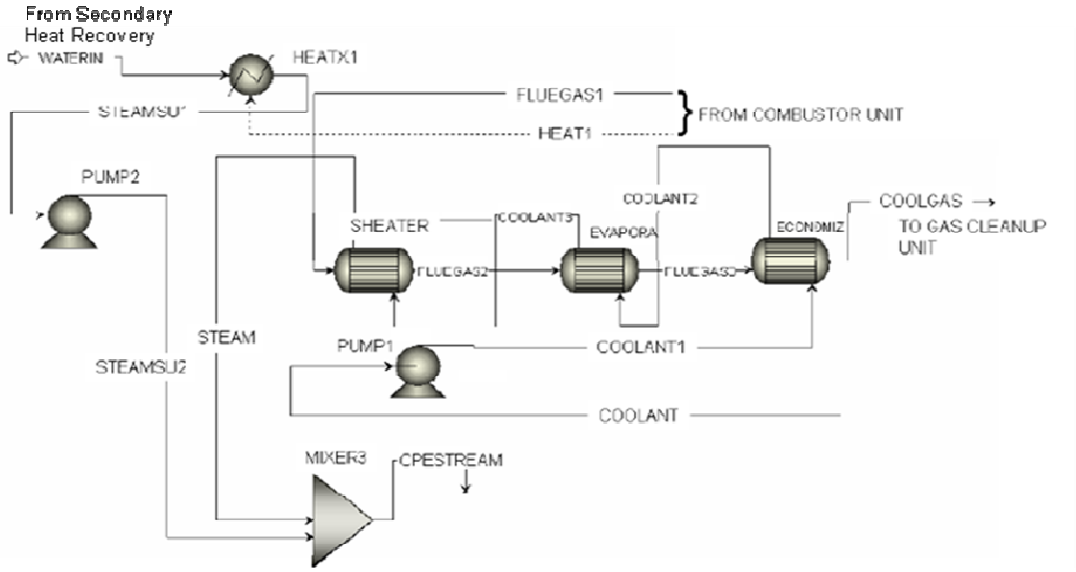

Fig. 3.5 – Flow diagram of steam recovery section

Table 3.5 Important parameters used for modeling the heat recovery section

Unit Operation	Modeling Parameters Used
HeatExchanger (ECONOMIZ)	Cold Stream Outlet Vapor Fraction = 0 Minimum Temperature Approach = 10°F
HeatExchanger (EVAPORA)	Cold Stream Outlet Vapor Fraction = 1 Minimum Temperature Approach = 10°F
HeatExchanger (SHEATER)	Cold Stream Outlet Temperature = 1100°F Minimum Temperature Approach = 10°F
Heater (HEATX1)	Pressure = 14.7 psia
Pump (PUMP2)	Discharge Pressure = 2175.56 psia
Mixer (MIXER3)	Pressure = 2175 psia

3.7 Modeling the Heat Recovery Unit (HRU) and Steam Generation

Power generation is modeled by Rankine cycle (Fig. 2.6). Steam that comes out of the heat recovery and secondary heat recovery sections is routed to the steam turbine of

the power generation section. The Rankine cycle consists of two steam turbines. One operates at a high-pressure of 174 psia and other operates at a low-pressure of 14.7 psia. The main advantage of using the Rankine cycle is its higher efficiency than other power generation cycles. This is because of the efficient use of the low-pressure steam. The steam coming out of the high-pressure steam turbine is split into two different streams. One is fed to the low-pressure turbine and other to the condensed liquid that comes out after passing through the low-pressure turbine and condenser.

The turbines are assumed to be isentropic with isentropic efficiency of 0.92 and mechanical efficiency of 0.95.[16] A mixer is used to mix both steam streams, one from the main heat recovery section and other from the secondary heat recovery section. The mixed steam stream then enters the high-pressure steam turbine modeled by a high-pressure turbine. Steam from the high-pressure turbine is split into two streams; one is fed into the low-pressure turbine and other is rerouted to a mixer. The steam that comes out of the low-pressure turbine enters the condenser. Cooled steam condensate coming out of the condenser is pumped to a discharge pressure of 174 psia. It is then mixed with the split stream from the high-pressure turbine using a mixer. The mixed steam stream is then recycled back to economizer. Fig. 3.6 and Table 3.6 are the flow diagram and unit operations used in the power generation section of the flow sheet.

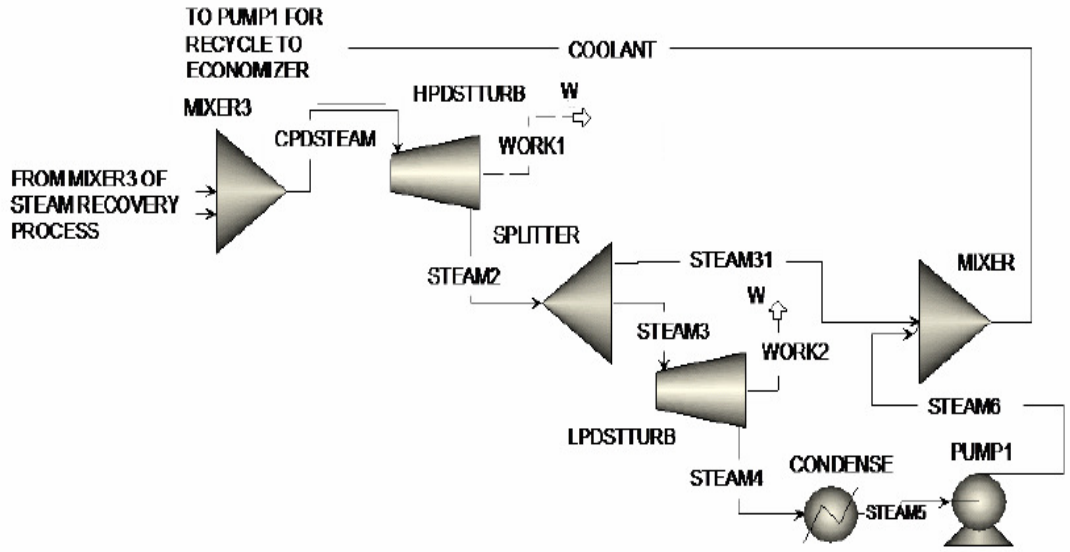

Fig. 3.6 - Flow diagram of a Rankine cycle

Table 3.6 Important parameters used for modeling the steam cycle section

Unit Operation	Modeling Parameters Used
Mixer (MIXER3)	Pressure = 2175 psia
Turbine (HPSTTURB)	Discharge Pressure = 174 psia Isentropic Efficiency = 0.92 Mechanical Efficiency = 0.95
Feed Splitter (SPLITTER)	Split Fraction of STEAM31 = 0.2368
Turbine (LPSTTURB)	Discharge Pressure = 14.7 psia Isentropic Efficiency = 0.92 Mechanical Efficiency = 0.95
Heater (CONDENSE)	Pressure = 14.7 psia Degrees of Sub-cooling = 0
Mixer (MIXER)	Pressure = 174 psia

3.8 Sulfur Removal Unit (SRU)

Flue gas from the boiler exit is cooled to moderate temperatures and the sulfur recovery unit removes the calcium sulfate from the gas. This is modeled by a settler that separates the solid calcium sulfate that condenses at lower temperature from the flue gas.

The flue gas that exits contains mainly CO_2, H_2O, O_2, N_2, and traces of SO_3 and NO_x gases.

3.8.1 Modeling the Sulfur Removal Unit (SRU)

Flue gas undergoes the heat recovery process and comes out of the heat recovery unit as cool gas, which flows into the sulfur separator. The sulfur separator operates at atmospheric conditions and separates the sulfate formed by the sulfate reactions described in section 2. Ninety nine percent of the calcium sulfate formed is removed by this separation process. Fig. 3.7 shows the sulfur removal unit.

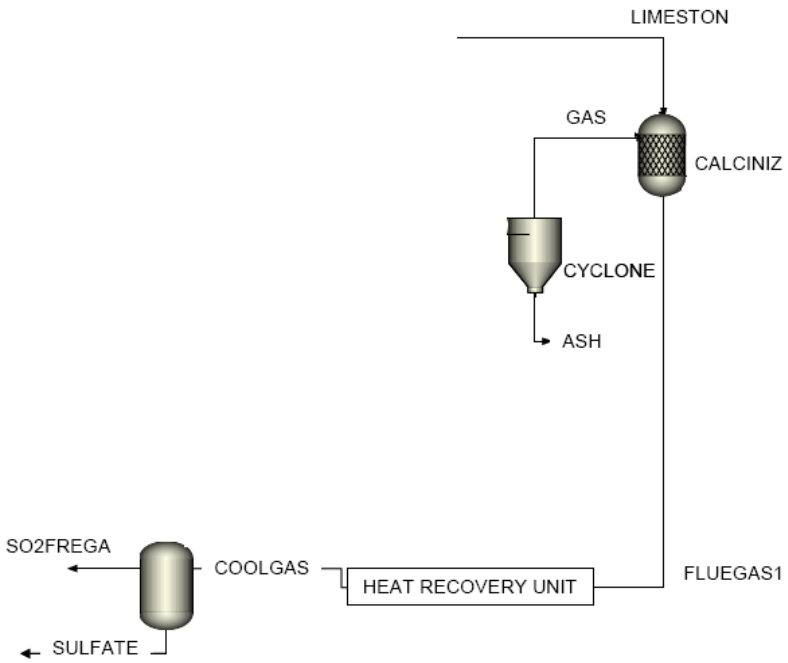

Fig. 3.7 - Flow diagram of sulfur removal section

3.8.2 NO_x Control

The quantitiy of NO_x gases in flue gas mainly depends on the amount of nitrogen initially present in the feedstock. The Tuscaloosa petcoke used in the modeling has 1.7 wt% of nitrogen. The amount of NO_x gas is very minimal in our case. To remove these NO_x gases, the gas can be scrubbed with water and nitric acid in the presence of a small amount of hydrogen peroxide. The reactions that take place during the process are given below [15]:

$$3NO_2 + H_2O \rightleftharpoons 2HNO_3 + NO \quad (26)$$

$$NO + HNO_3 + H_2O \longrightarrow 3HNO_2 \quad (27)$$

$$HNO_2 + H_2O_2 \longrightarrow HNO_3 + H_2O \quad (28)$$

These reactions are generally fast and the gas that comes out the process is free of NOx pollutants. Since NO_x gases coming out of combustor is negligible, nitrogen oxide removal process was not modeled.

4. MODELING THE GASIFICATION PROCESS

The gasification process is explained in this section. The gasification process is divided into five main sections: gasification island, gas cooling, gas cleanup, gas turbine section and steam cycle.

4.1 Overall Process Flow Description

A typical process flow diagram of an IGCC process has already been shown in Fig. 2.7 in section 2. Feedstock is prepared and fed into the gasifier along with steam and oxygen. Gasification reactions take place at high temperature in the range of 2,000^{o}F to 2,700^{o}F.[2] The heat recovery unit in gasification is modeled with two methods namely: radiant -convective cooling and direct quenching is employed for heat recovery. Gas cleanup follows the cooling process, in which sulfur is removed by a Claus process. Claus process is an efficient method for removing hydrogen sulfide in the syngas by converting it into elemental sulfur. The main reactions that take place in a Claus furnace are:[26]

$$2\,H_2S + O_2 \rightarrow 2S + 2H_2O \qquad (29)$$

$$2\,H_2S + 3O_2 \rightarrow 2SO2 + 2H_2O \qquad (30)$$

$$2\,H_2S + SO_2 \rightleftharpoons 3S + 2H_2O \qquad (31)$$

Cleaned gas is then sent to the combined cycle section consisting of gas and steam turbine for further power generation.

4.2 Gasification Island

The gasification island includes feedstock preparation and the gasifier. Solid fuels such as petcoke are crushed finely to improve burning efficiency during gasification. The petcoke is then fed into the gasifier along with steam and oxidant. In the gasification process, oxygen with purity of 95 mol% is used as the oxidant. Oxygen of 95 mol% purity is prepared by an atmospheric separation unit (ASU). Oxygen is compressed to a pressure closer to the operating pressures of the gasifier. Steam is also fed as a feed material. The feedstock forms slurry before it enters the reactor. When fed into the reactor, petcoke decomposes into its elemental components based on the ultimate analysis of the feedstock.

The gasification process is as fast as the combustion process, with mean residence times from 0.4 to 5 seconds.[2] Since the reaction is fast, we modeled it with simple reactions involving gasification of elemental components. The ultimate and proximate analyses of the petcoke used in the modeling have been described previously.

4.2.1 Modeling the Gasification Island

Similar to the combustion process, feedstock is crushed to a uniform size before it is fed into the reactor. Crushing facilitates solids handling and improves the efficiency of gasification. If the feedstock is fed into the gasifier as lumps, overall gasification efficiency decreases and the amount of un-reacted feedstock coming out of the reactor is high. In the IGCC process, the feedstock is fed with steam and oxidant. The petcoke

from the crusher is fed into the gasification reactor. This reactor is modeled by a two-stage process with a yield reactor followed by equilibrium reactor. The yield reactor virtually breaks the non conventional petcoke feedstock into its constituent elements. Petcoke that comes out of the decomposition reactor flows into the equilibrium reactor. The gasifier was modeled using equilibrium reactions. The oxidant, which consists of 95 mol% O_2 and 5 mol% N_2, enters the gasifier for the gasification reactions to take place along with a separate stream of steam. The oxidant stream is pressurized to a pressure of 610 psia. This is done to achieve a pressure range closer to that of steam, which enters the gasifier at a temperature of 487^{o}F and a pressure of 600 psia. The pressure was selected based on the emission components and mixture composition coming out of the gasifier.

Gasification reactions in the gasifier are modeled by identifying the possible products. The products that are likely to be formed in a gasification reaction were entered as the main parameters for the gasifier. The gasification reactions are assumed to take place at a temperature of 2,552^{o}F. This temperature was based on a sensitivity analysis within the temperature range for the gasification reaction of 2,200 to 2,700^{o}F. The temperature showed maximum CO and H_2 concentration at that temperature with lowest emissions compounds like sulfur trioxide and H_2S. (This is described in detail in the following section.) Once the gasification process is complete, the syngas is fed into cyclone separators to remove ash.[25] The ash free gas then flows into the gas cooling

section. Fig. 4.1 shows the typical flow diagram of gasification island. The main unit operations modeled in the gasification island are described in Table 4.1.

Table 4.1 Important parameters used for modeling the gasification island section

Unit Operation	Important Parameters Used
Pump (GSPUMP)	Pressure = 435 psia Isentropic Efficiency = 0.92
Heat Exchanger (BOILER)	Pressure = 600 psia Temperature = 487^{o}F
Pressure Changers (GSCOMPRE)	Pressure = 610 psia Isentropic Efficiency = 0.92
Stoichiometric Reactor (DECOMPS)	Pressure = 600 psia Temperature = 77^{o}F
EQUILIBRIUM (GSGASIFI)	Pressure = 610 psia Temperature = 2552^{o}F
Cyclone (ASHREM1)	Efficiency Correlation = Leith - Licht Diameter = 0.5m
Cyclone (ASHREM2)	Efficiency Correlation = Leith – Licht Diameter = 0.1m

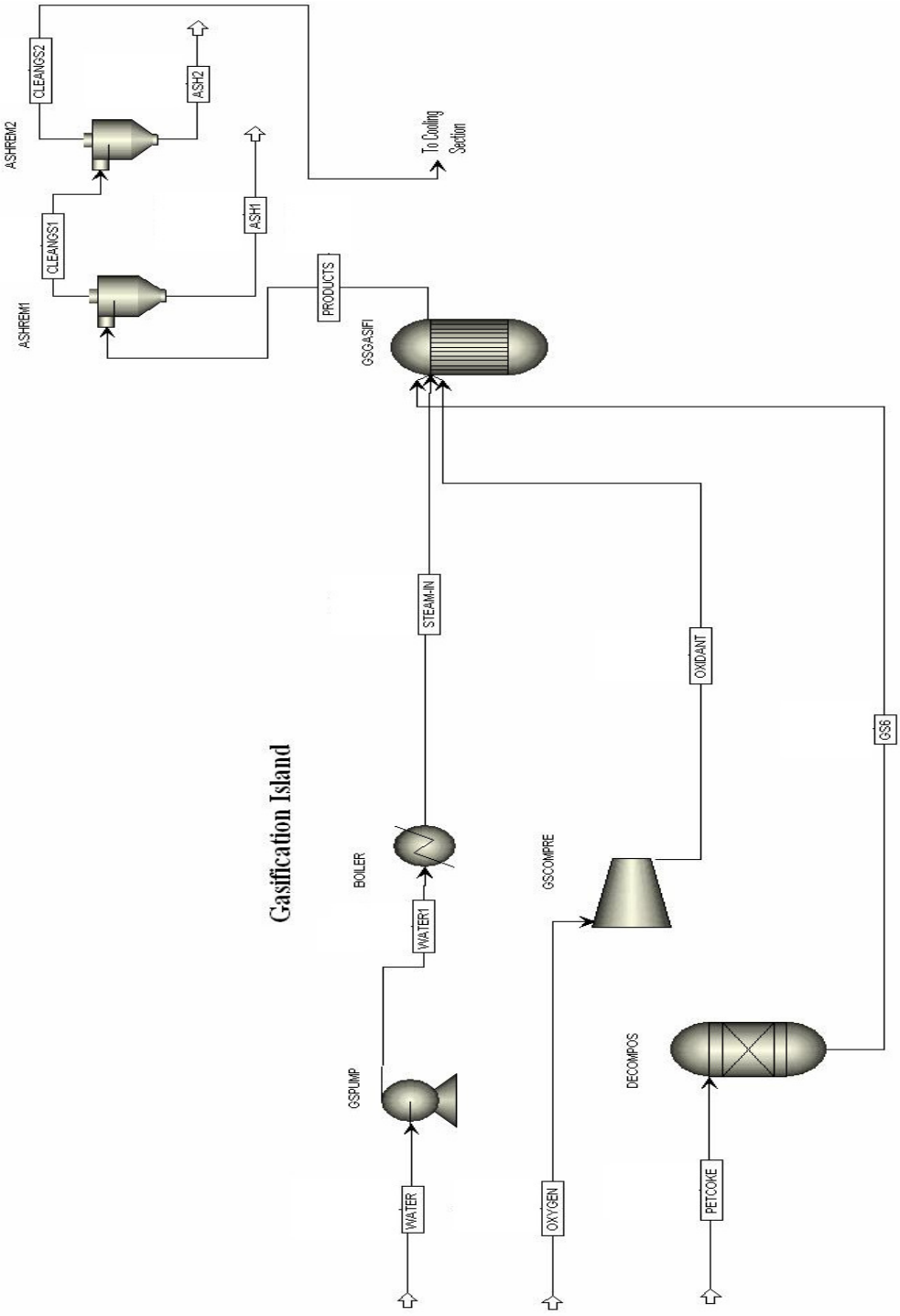

Fig. 4.1 Flow diagram of gasification island section

4.3 Gas Cooling

Gas cooling is an important heat recovery process in gasification. Gas cooling is done by two popular methods: the radiant/convective cooling method and the total quench method. In the radiant - convective method the raw syngas that comes out of the gasifier at high temperature is cooled to a moderate temperature of 500^{o}F by a three-step process, whereas in the total quench design the raw syngas is cooled directly to around 500^{o}F in a single step. Water is commonly used for quenching the heat. In the model, raw syngas that comes out at an elevated temperature of around 2,500^{o}F is cooled to a temperature of 500^{o}F by a three-step cooling process[2, 25].

4.3.1 Modeling the Gas Cooling

The raw syngas that comes out of the gasifier is at very high temperature and is cooled by a three-step process. Using a series of coolers reduces the temperature of the raw syngas from 2,552^{o}F to 500^{o}F. These heat recovery boilers generate steam that is redirected to the mixer, which acts as a coupling unit for different steam streams. Steam is redirected to the heat recovery steam generation (HRSG) section. Cooled syngas is fed into the separator, which removes traces of ash and other particulate matter. Fig. 4.2 is a typical flow diagram of our modeled gas cooling and ash removal area. The main unit operations modeled in the gas cooling and ash removal are described in Table 4.2.

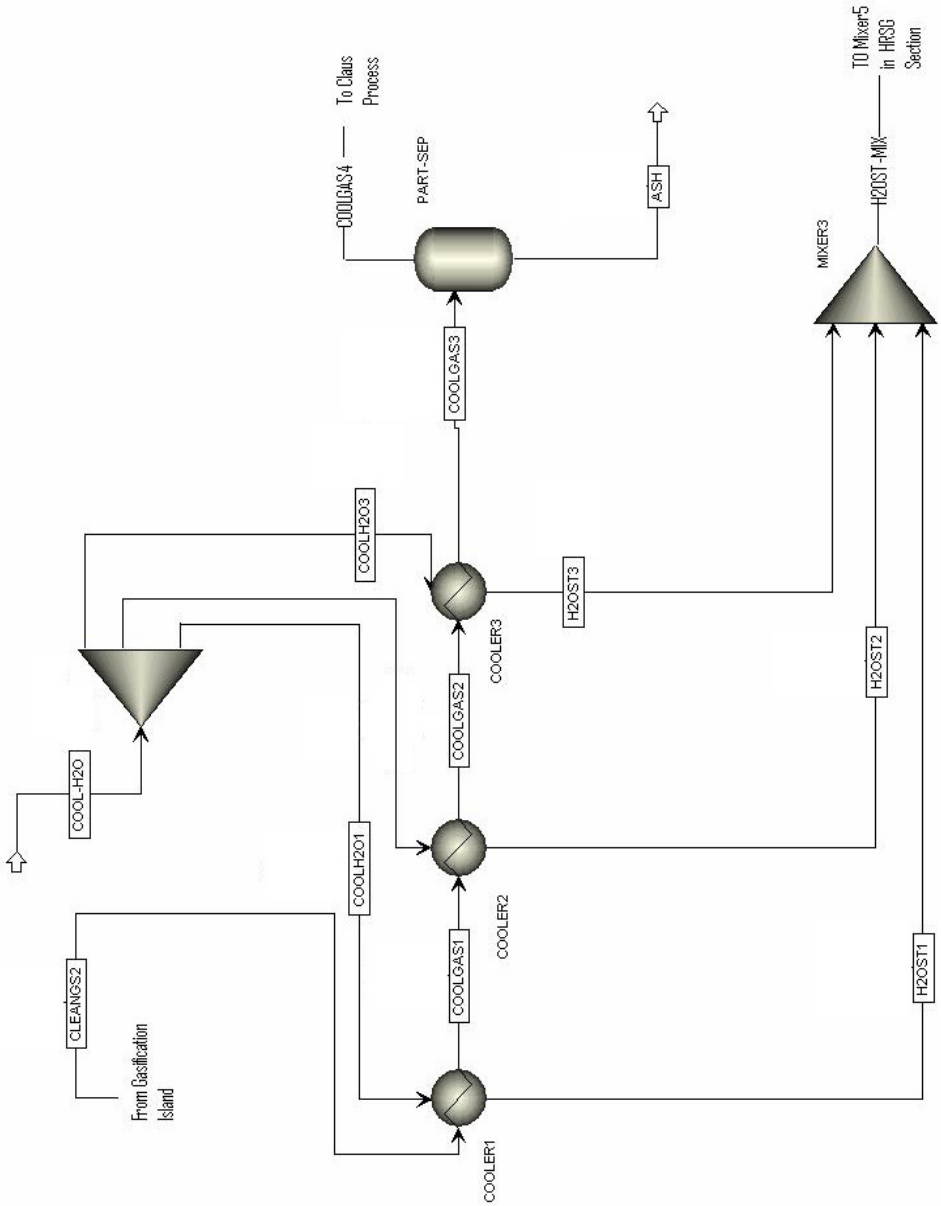

Fig. 4.2 Flow diagram of gas cooling section

Table 4.2 Important parameters used for modeling the gas cooling section

Unit Operation	Important Parameters Used
Heat Exchanger (COOLER1)	Operating Pressure = 600 psia Outlet Temperature = 1500^{o}F
Heat Exchanger (COOLER2)	Operating Pressure = 600 psia Outlet Temperature = 750^{o}F
Heat Exchanger (COOLER3)	Pressure = 600 psia Outlet Temperature = 500^{o}F

4.4 Gas Cleanup

Gas cleanup is a general term for removing particulate impurities such as ash, soot and acid gas (H_2S). The gas that comes out of the gasifier has particulate matter like ash and soot. Cyclones are used to remove the particulate matter. H_2S is selectively converted to elemental sulfur by the Claus process. The Claus process is efficient method in which 98% of the H_2S is converted to elemental sulfur.[26]

4.4.1 Modeling the Gas Cleanup

Gas cleanup mainly involves the removal of sulfur by the Claus and Selexol process. The selexol separator is a packed-bed column, mainly to separate acid gas from the gas stream. The Claus process mainly involves the conversion of H_2S gases into elemental sulfur. The Claus process involves multistage catalytic oxidation of H_2S following the overall reaction,

$$2\ H_2S + O_2 \rightarrow 2S + 2H_2O \qquad (32)$$

The Claus process involves burning one-third of the H_2S with air in a reactor furnace to form sulfur dioxide (SO_2) according to the following reaction,

$$2H_2S + 3O_2 \rightarrow 2SO_2 + 2H_2O \qquad (33)$$

The normal operating range of the Claus furnace is from 1,800 to 2,800°F with pressures slightly higher than atmospheric. The gas then enters a heat exchanger where the heat is recovered. Sulfur condenses through the separator and almost 60 to 65% of sulfur is recovered by this process. The steam generated by the heat exchanger is redirected to the HRSG where it can be used. The gas stream then enters the Claus separator where converted sulfur is recovered with 99% efficiency, and then fed into the Claus reactor, where the remaining two-thirds of the unreacted hydrogen sulfide is converted to sulfur by the following reaction,

$$2\,H_2S + SO_2 \rightleftharpoons 3S + 2H_2O \qquad (34)$$

Claus separation was modeled at an operating temperature of 360°F and 10 psig. The recovery of this stage is also around 98 to 99%. A sulfur free stream of syngas enters the gas turbine section for further power generation. Fig. 4.3 shows the typical flow diagram of the Claus process. The main unit operations modeled in the Claus process are described in Table 4.3.

Table 4.3 Important parameters used for modeling the gas cleanup section

Unit Operation	Important Parameters Used
Reactor (CFURNACE)	Pressure = 24.7 psia Operating Temperature = 2012^{o}F
Heat Exchanger (COOLER5)	Pressure = 24.7 psia Outlet Temperature = 240^{o}F
Separator (CLAUSSP1)	Pressure = 24.7 psia
Heat exchanger (CLAUSHR2)	Pressure = 24.7 psia Outlet Temperature = 495^{o}F
Reactor (CFURNAC2)	Pressure = 24.7 psia
Separator (CLAUSSP2)	Pressure = 24.7 psia
Heat Exchanger (REHEATER)	Outlet Pressure = 250 psia Outlet Temperature = 700^{o}F

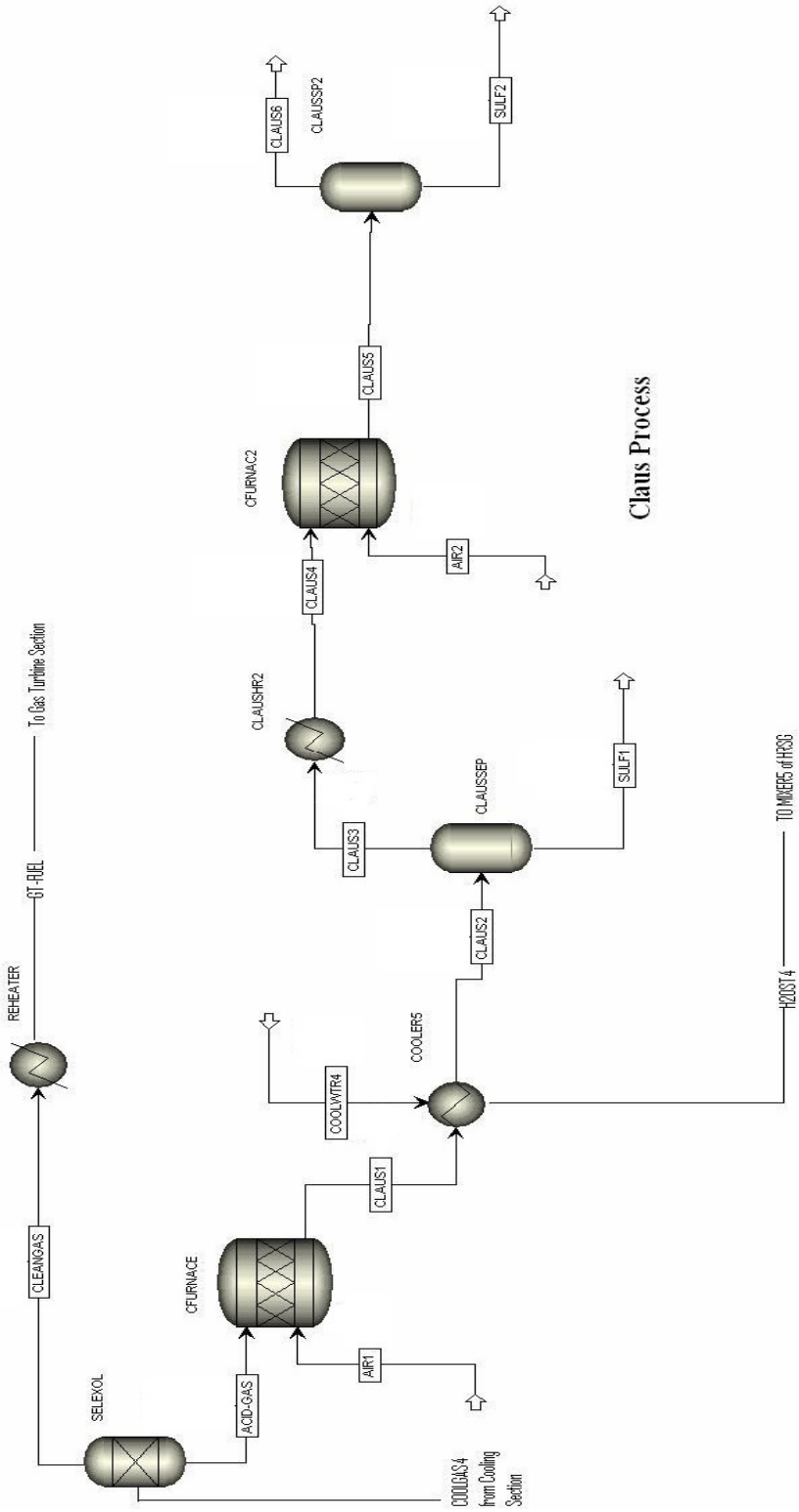

Fig. 4.3 Flow diagram of Claus process section

4.5 Gas Turbine Section

The gas cycle is modeled using the Brayton cycle.[16] Gas turbines are sensitive to sulfur-bearing pollutants. Therefore, sulfur compounds are removed prior to the gas turbine cycle. Cleaned syngas is then fed into the combustor of the gas turbine cycle, where combustion reactions take place. This helps to drive the gas turbine that forms a part of combined cycle.[16]

Cooled sulfur-free syngas then enters the gas turbine section. Air and nitrogen also enter the gas turbine compressor, which is modeled as is three stages with compressors. The gas is compressed to pressures 10 times higher than the atmospheric pressure.[2, 16] The compressed gas stream then flows into the gas turbine combustor. The combustor is modeled using a stoichiometric reactor. The products of incomplete combustion undergo complete combustion in the combustion furnace. Products of combustion in the gas turbine cycle then enter the three-stage gas turbine unit. Exhaust gas coming out of gas turbine section is routed to the HRSG section for generating steam through heat recovery. The isentropic efficiency for the compressors and expanders were assumed to be 92%, as cited in the literature.[16] Fig. 4.4 shows a typical flow diagram of the gas turbine section modeled in Aspen. The main unit operations modeled in the gas turbine cycle is described in Table 4.4.

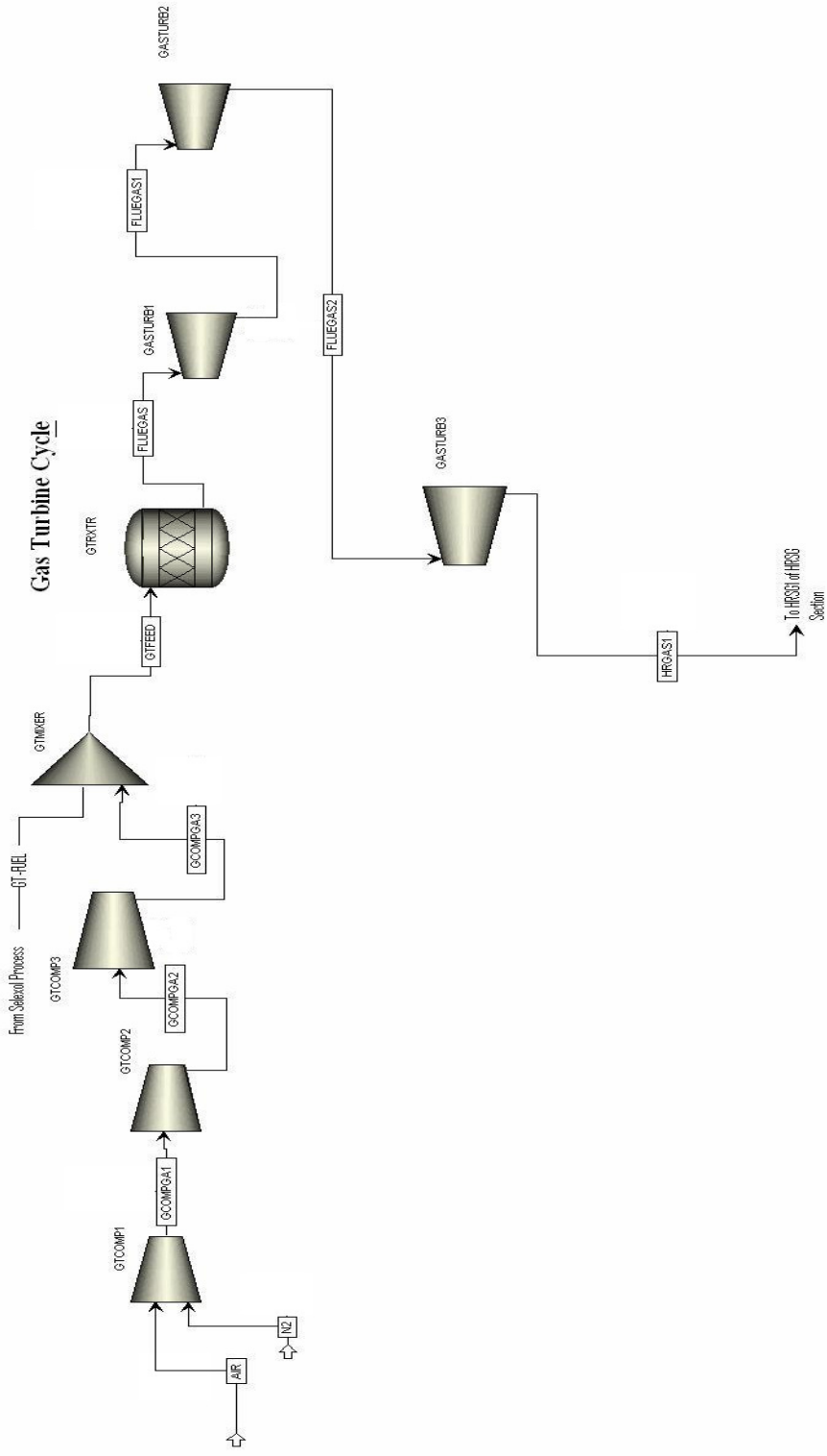

Fig. 4.4 Flow diagram of gas turbine section

Table 4.4 Important parameters used for modeling the gas turbine section

Unit Operation	Important Parameters Used
Compressor (GTCOMP1)	Outlet Pressure = 50 psia Isentropic Efficiency = 0.92
Compressor (GTCOMP2)	Outlet Pressure = 150 psia Isentropic Efficiency = 0.92
Compressor (GTCOMP3)	Outlet Pressure = 250 psia Isentropic Efficiency = 0.92
Reactor (GTRXTR)	Pressure = 206 psia Temperature = 2200^{o}F
Expander (GASTURB1)	Outlet Pressure = 100 psia Isentropic Efficiency = 0.92
Expander (GASTURB2)	Outlet Pressure = 50 psia Isentropic Efficiency = 0.92
Expander (GASTURB3)	Outlet Pressure = 14.7 psia Isentropic Efficiency = 0.92

4.6 Steam Cycle

The steam cycle consists of two main sections: the heat recovery steam generator (HRSG) and steam turbine. The HRSG which consists of reheaters and boilers acts a common pool for coupling various heat streams. This unit superheats saturated steam and sends it to the steam turbine section, where it is expanded to generate power. The steam cycle is modeled based on the Rankine cycle. The gas turbine and steam turbine constitute the combined cycle. The total shaft work to the generator is provided by both gas turbine and steam turbine.[16]

4.6.1 Heat Recovery Steam Generation (HRSG)

The heat recovery steam generator is modeled by two heat-recovery units. These two units generate steam from the gas stream that exits the gas turbine section. The steam

generated from the heat-recovery units is redirected to boiler of steam turbine section, where steam is generated using boiler feed water.

4.6.2 Steam Turbine Section

Power generation in the steam turbine section was modeled using the Rankine cycle. The steam from the HRSG is routed to the reboiler. Steam that comes out of the HRSG and auxiliary heat streams are routed to the steam turbine of the power generation section. The steam cycle is modeled with a high-pressure turbine and a low-pressure turbine. The high-pressure turbine operates at 174 psia and the low-pressure turbine operates at a low-pressure of 14.75 psia. The pressures are chosen on the basis of expansion that could result in maximum power output. The analysis of selection of our selection of the optimum pressure is discussed in detail in the next section.

The turbines are assumed to be isentropic to model the way used in the Texaco gasification process with isentropic efficiency of 0.92. A mixer is used to mix the steam streams, one from the heat recovery section and the other from secondary heat recovery section. The mixed steam stream then enters the high-pressure steam turbine. The steam stream from the high-pressure turbine is split into two streams; one is fed into the low-pressure turbine and other stream is rerouted to the mixer. The steam which comes out of the low-pressure turbine enters the condenser. The cooled steam condensate coming out of the condenser is pumped to a discharge pressure of 174 psia. It is then mixed with the split stream from the high-pressure turbine using a mixer. Mixed steam stream is then

recycled back to the economizer. Fig. 4.5 and Table 4.5 describe the flow diagram and unit operations used in the steam power generation section of the flow sheet.

Table 4.5 Important parameters used for modeling the steam turbine section

Unit Operation	Important Parameters Used
Heat Exchanger (HRSG1)	Temperature = 750^{o}F
Heat Exchanger (HRSG2)	Temperature = 550^{o}F
Heat Exchanger (REBOILER)	Temperature = 1112^{o}F Pressure = 2175 psia
Compressor (HPSTTURB)	Discharge Pressure = 174 psia Isentropic Efficiency = 0.92 Mechanical Efficiency = 0.95
Compr (LPSTTURB)	Discharge Pressure = 14.7 psia Isentropic Efficiency = 0.92 Mechanical Efficiency = 0.95
Heater (CONDENSE)	Pressure = 14.7 psia Degrees of Sub-cooling = 0
Mixer	Pressure = 175 psia
Pump (PUMPI)	Discharge Pressure = 175 psia

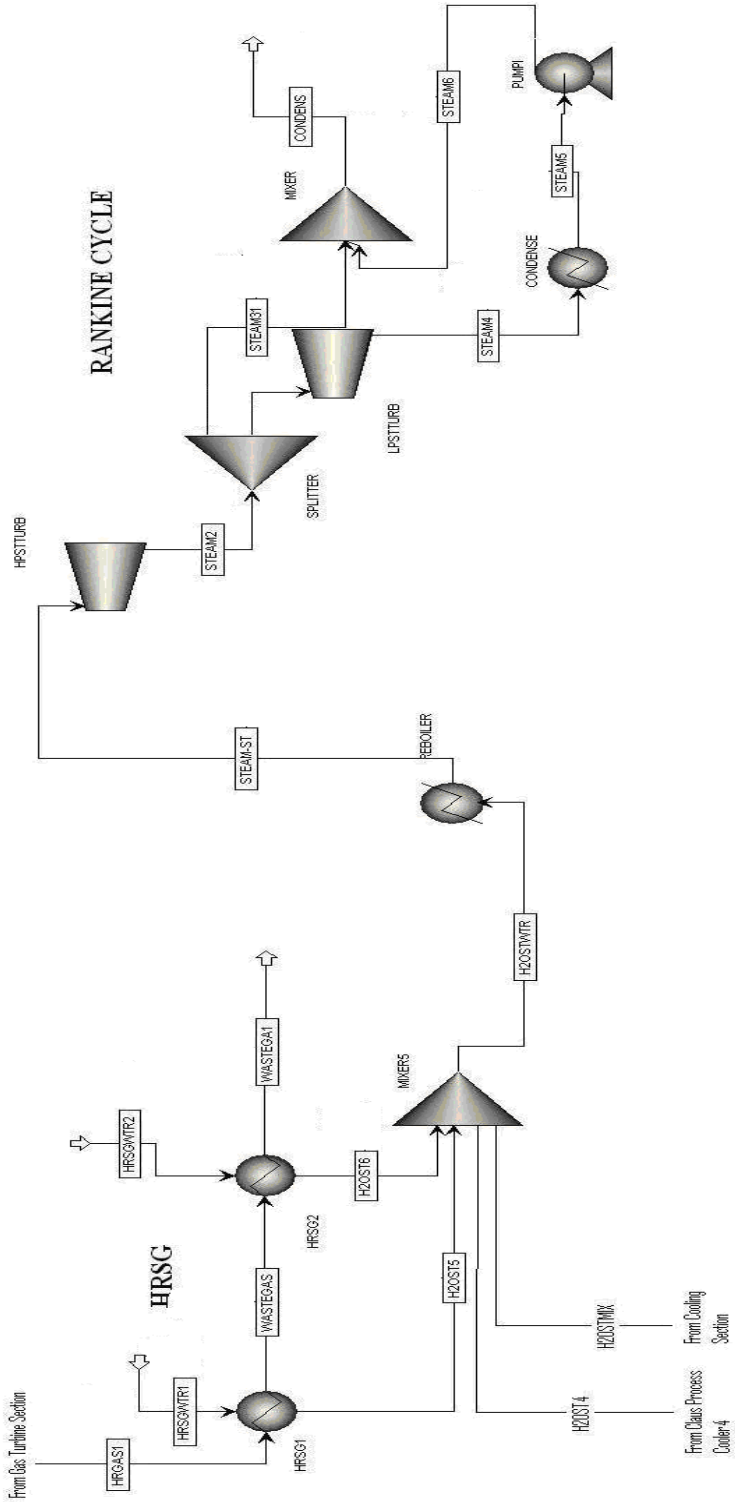

Fig. 4.5 – Flow diagram of steam turbine section

5. SENSITIVITY AND EMISSION ANALYSIS OF THE PROCESSES

Sensitivity analysis of both processes is discussed in detail in this section. Both processes have certain parameters such as temperature, pressure, and flow rate of steam and oxidant that control the overall efficiency. The sensitivity analysis was carried out by varying these parameters within the range cited in the literature.

5.1 Sensitivity Analysis of Gasification Process

The sensitivity analysis in the gasification process was done by focusing on the gasifier, and the gas and steam turbine parameters that have a notable effect on power generation. These parameters include temperature, pressure of the gasifier, oxygen flow rate, steam rate, and gas turbine discharge pressure conditions.

5.1.1 Temperature Variation

Temperature variation was aimed mainly at the final composition of the syngas coming out of the gasifier. Compositions of CO and H_2 in syngas were monitored to determine the initial temperature. In general, the gasifier operates in the range of 1,800 – 2,500^{o}F. Variation of syngas composition was analyzed in this range. Fig. 5.1 shows the variation of carbon monoxide and Fig. 5.2 shows the variation of hydrogen with temperature.

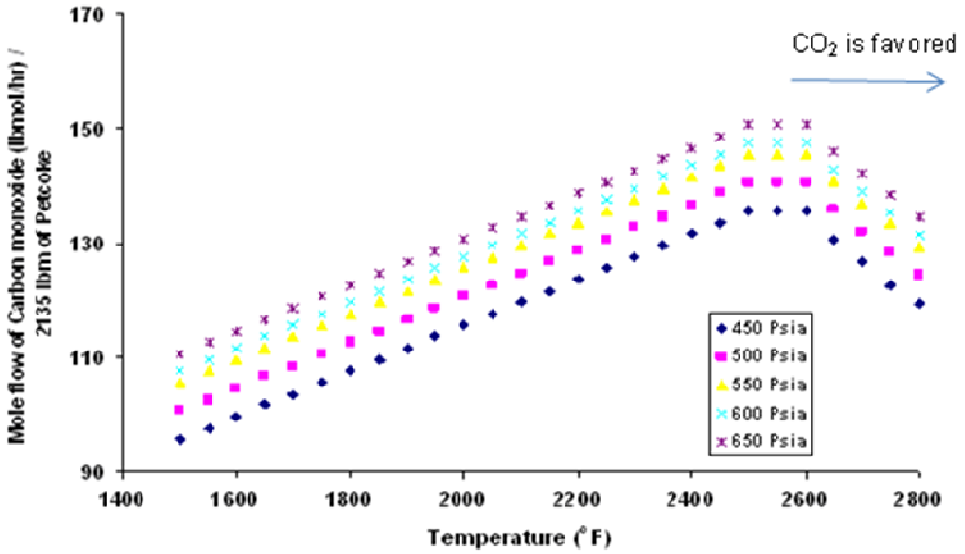

Fig. 5.1 - Carbon monoxide variation with temperature

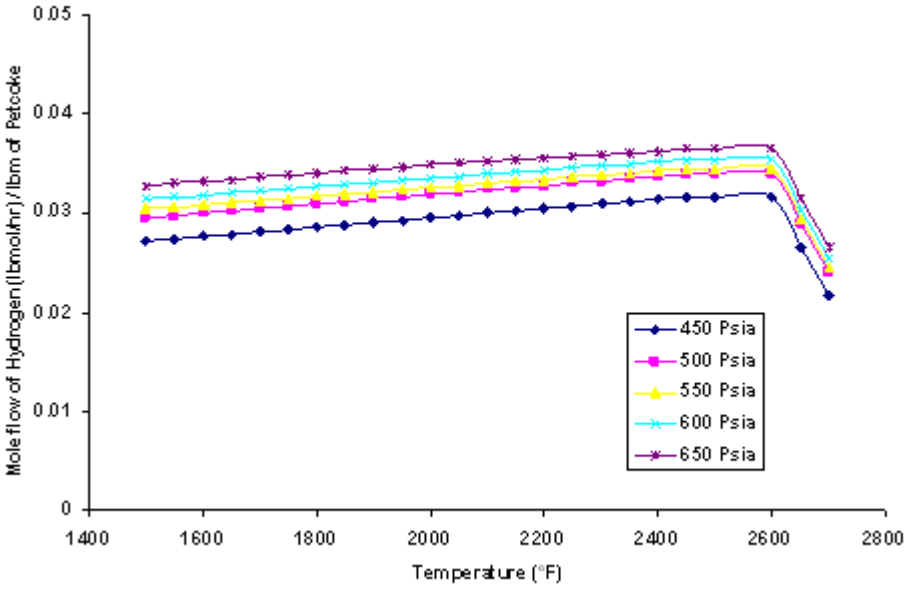

Fig. 5.2 - Hydrogen flow rate variation with gasification temperature

From Figs. 5.2 and 5.3 we can clearly see that at around 2,550^{o}F both carbon monoxide and hydrogen attain maximum concentration in the syngas. At very high temperatures (around 2,700 – 2,800^{o}F) the concentration of carbon monoxide and hydrogen starts decreasing. This is because both carbon monoxide and hydrogen are unstable at high temperatures and convert into completely combustible products such as CO_2 and H_2O if the oxygen supply is sufficient. H_2S, is the main harmful effluent which comes out of the gasifier, also varies with increase in temperatures. Fig. 5.3 shows the variation of hydrogen sulfide with temperature.

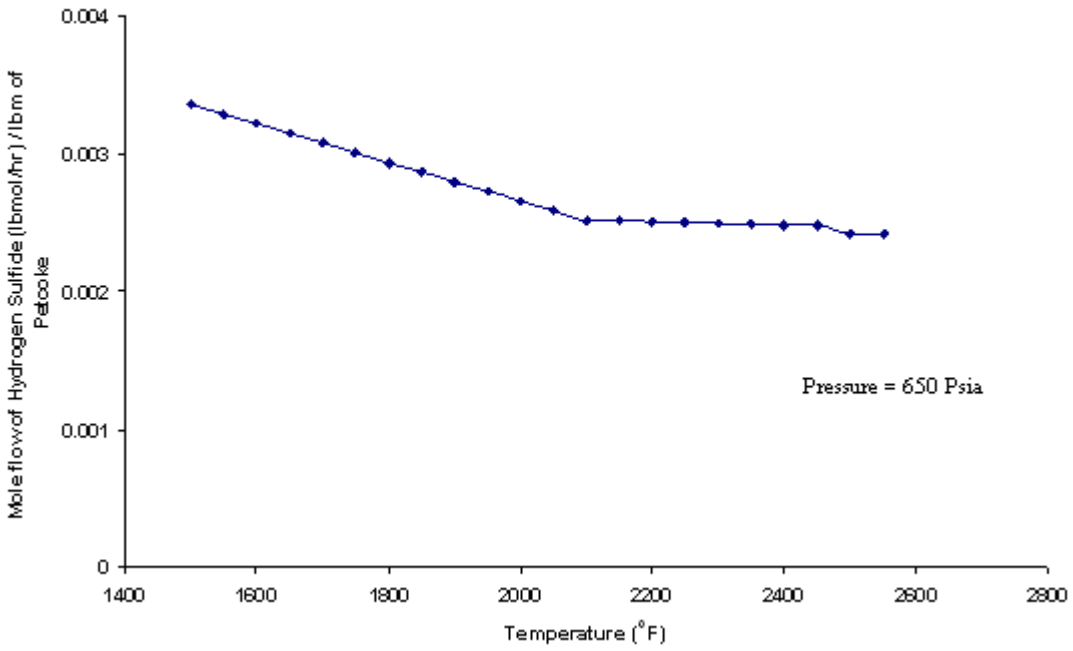

Fig. 5.3 - Hydrogen sulfide flow rate variation with gasification temperature

5.1.2 Pressure Variation

Pressure variation was aimed at minimizing the volume of gas coming out of the gasifier. In general, Texaco gasifiers operate at high-pressure around 400 to 650 psia. A sensitivity analysis was performed within this range to analyze the volume of the gas. Since gas turbines operate better with low volumetric flow rates, pressure of 650 psia was selected to be the operating pressure. Operating with high volumes of gaseous products in gas turbines subsequently increases the capital and operating cost. Hence high pressure is preferred in gas turbines to reduce the volume and also to decrease costs involved in handling large volumes of gas.

5.1.3 Oxygen Variation

Oxygen variation was aimed at maximizing the flow rate of the carbon monoxide and hydrogen mixture and at minimizing the flow rate of the completely combustible products, carbon dioxide and water vapor. Fig. 5.4 shows the variation of the volumetric flow of the individual components (carbon monoxide, hydrogen, carbon dioxide and water vapor) with the oxygen flow rate. Thus, maximizing the flow rate of carbon monoxide and hydrogen in the syngas stream increases the heat content of the outlet stream, which in turn increases the power generation from gas turbine during combustion of syngas.

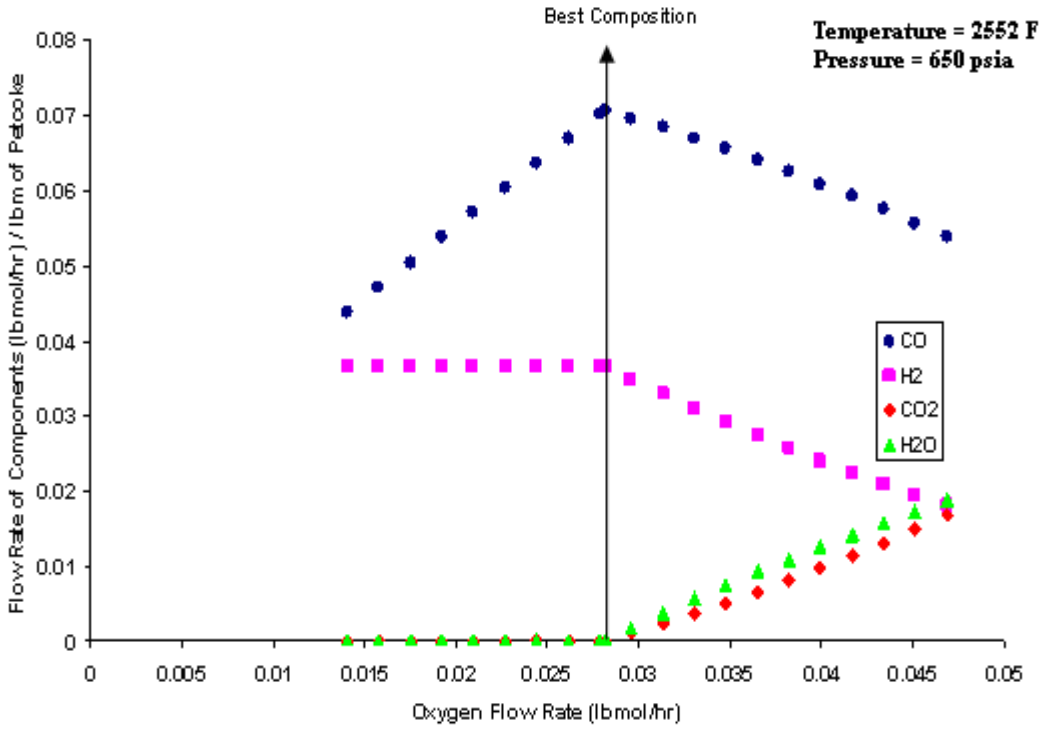

Fig. 5.4 – Flow rate of components with variation in oxygen in the gasification

5.1.4 Steam Variation

Similar to oxygen variation, steam sensitivity analysis was aimed at achieving a higher flow rate of carbon monoxide and hydrogen in the outlet stream. Fig. 5.5 shows the variation of volumetric flow of carbon monoxide, hydrogen, carbon dioxide and water vapor with the steam flow rate. Optimum steam flow rate for the given petcoke flow rate can be determined from the analysis, which was chosen again based on the maximum concentration of CO and H_2 in the syngas.

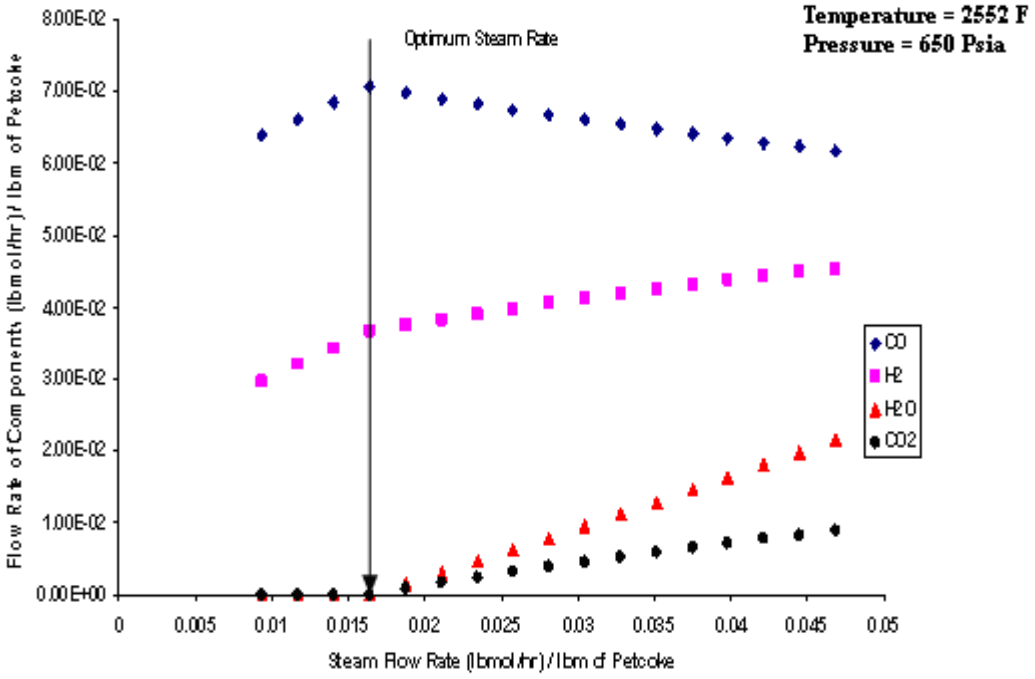

Fig. 5.5 Flow rate of components with variation in steam in the gasification

5.1.5 Steam Turbine Pressure Variation

Steam turbine expansion pressures determine the amount of power generated in the steam cycle. Sensitivity analysis was performed on steam turbine outlet pressure to determine the optimum values. From Fig. 5.6 we can observe that steam turbine power output increases for a given amount of steam flow, because of the high enthalpy drop in steam turbines. This is clearly prominent in a low-pressure steam turbine than a high-pressure one. The high-pressure steam turbine variation was varied between 105 to 550 psia. The optimum pressure from the graph can be determined as 105 psia. Low-pressure steam turbine variation was analyzed from 14.7 psia to 100 psia; the optimum pressure

was found to be around 30 psia. The low-pressure steam turbine should not drop below 23 psia because the enthalpy drop available becomes very small and volume flow becomes very large.[27]

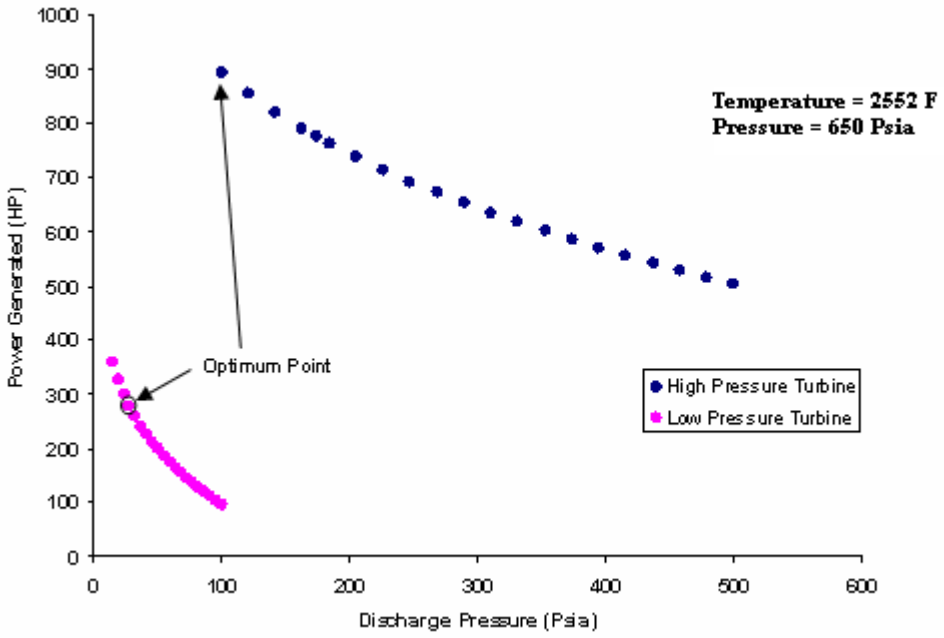

Fig. 5.6 – Power generation variation to steam turbine discharge pressures

5.2 Sensitivity Analysis of Combustion Process

Sensitivity analysis in the combustion process focused on the combustor parameters that have a notable effect on power generation. The temperature and air flow rate play

major roles in determining the combustion efficiency. The sensitivity analysis with variation to these parameters is shown below.

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5.2.1 Sensitivity to Air Rate

Sulfur dioxide and sulfur trioxide emissions are greatly influenced by the amount of excess air used. Air quantity was varied from 100% to 125% of the stoichiometric amount of air required for combustion. The air supplied was then denoted in terms of air/feedstock ratio. The variation in amount of SO_2 and SO_3 produced with variation in air/feedstock ratio is shown in Fig. 5.8. We can infer that sulfur dioxide formation decreases with increasing air rate while the sulfur trioxide level increases with decreases in the production of sulfur dioxide. We can see a slight variation in slope at 102%, corresponding to the stoichiometric amount of air required for the complete combustion to occur. This can be clearly seen in Fig. 5.7.

The sulfur dioxide produced during the combustion process reacts with the calcium oxide to produce calcium sulfate. The sulfur trioxide formed doesn't react with the calcium oxide, and should be minimized in the flue gas because it is known to produce acid rain. Because sulfur trioxide formation increases as the air supply is increased, the stoichiometric air supply of 102% was assumed in the process to minimize the emission of SO_3 in the flue gas. As a validation in the simulation process, emission of SO_3 was nearly equal to zero.

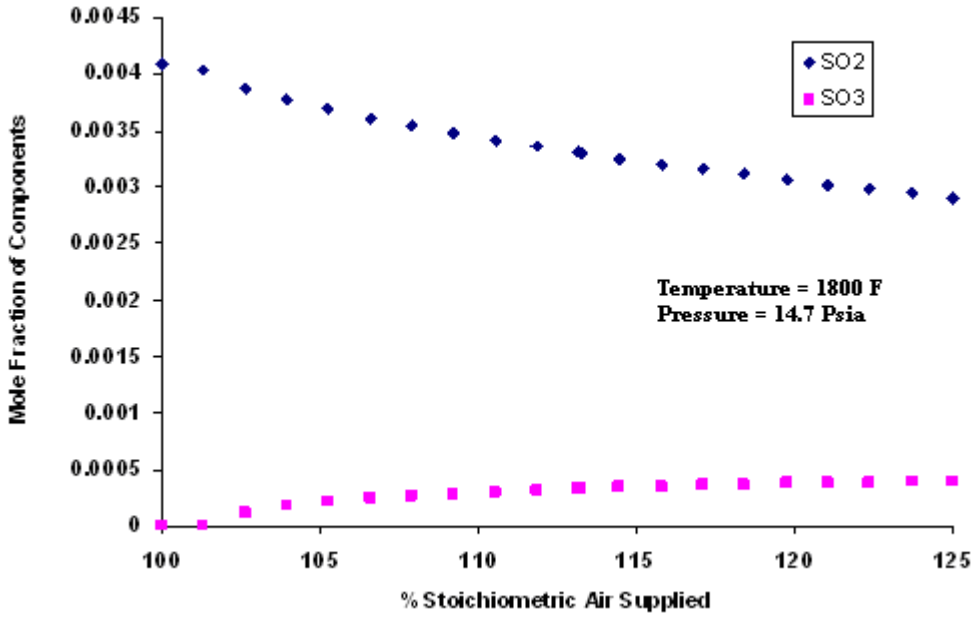

Fig. 5.7 – Sulfur oxide flow rate with air in the combustion process

Fig. 5.8 shows the amount of CO_2 produced with the air supplied. As expected, the produced CO_2 reaches its maximum value at the stoichiometric amount of air required for complete combustion.

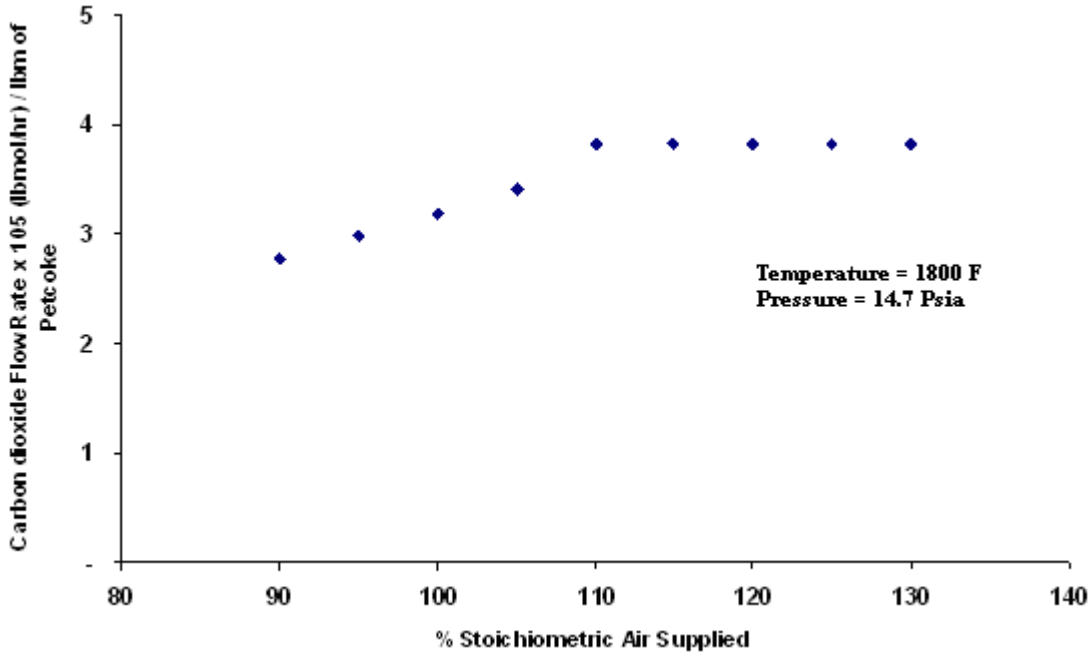

Fig. 5.8 - Carbon dioxide flow rate with air in the combustion process

5.2.2 Sensitivity to Temperature

Temperature plays an important role in the combustion process. Sensitivity analysis was analyzed with variation in temperature from 1,200^{o}F to 1,800^{o}F. Fig. 5.9 shows the amount of SO_x produced with variation in temperature.

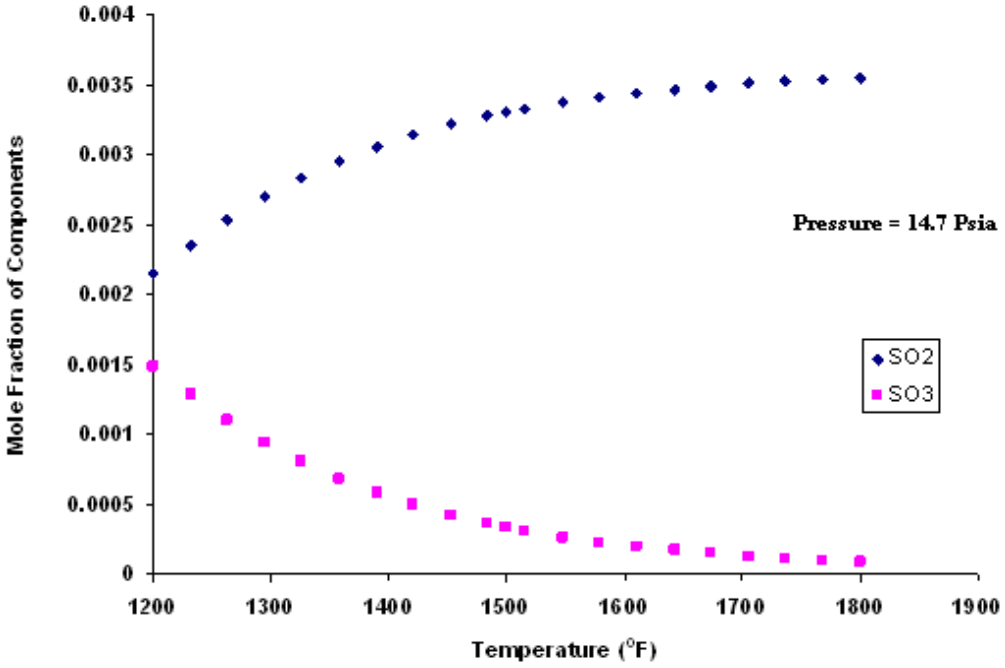

Fig. 5.9 - Sulfur oxide emission with temperature in the combustion process

We observe from the plot that the amount of sulfur dioxide formed increases with increase in temperature, whereas formation of sulfur trioxide decreases with temperature. This is because sulfur dioxide is more stable than sulfur trioxide at higher temperatures. Fig. 5.10 shows that the process efficiency decreases with temperature. This is because at high temperatures the available heat duty decreases and thereby decreases the combustion efficiency. However, higher temperature minimizes SO_3 emission. As a result, we use 1,800°F was used for the operating temperature, and after considering the entire power load of the utilities, the overall process efficiency was 32%. The equation used for calculating the efficiency is given as:

$$\eta_{Overall} = (W_{NE} \times 3600 \times OH) / (\dot{m}_{Petcoke} \times LHV_{Petcoke}) \qquad (35)$$

Computation of the efficiency calculation is discussed later in this section.

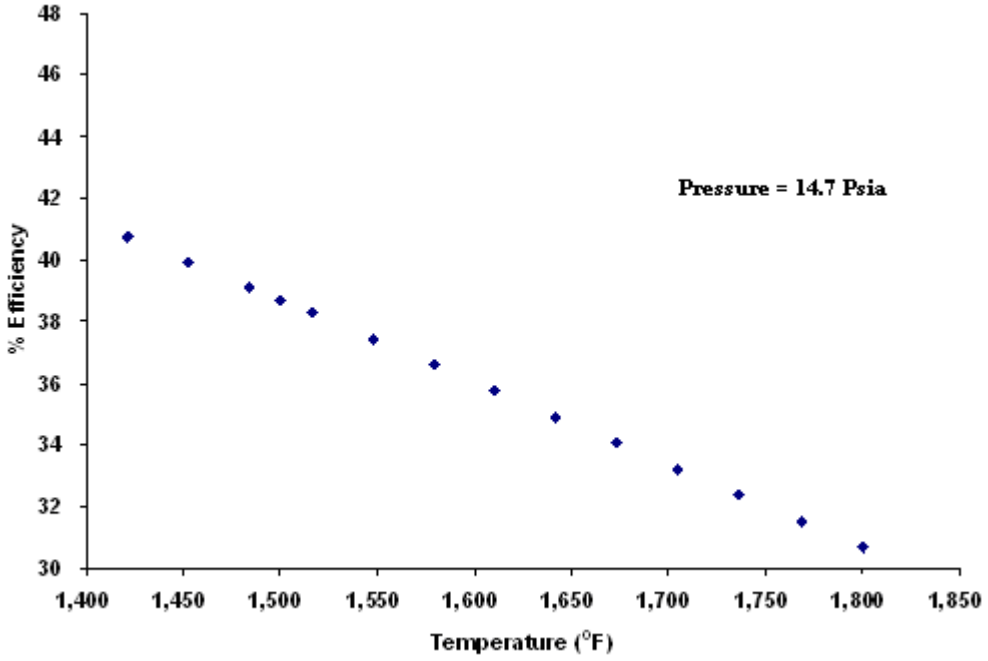

Fig. 5.10 - Efficiency of combustion process with temperature

Fig. 5.11 shows the increase in available heat load with variation in temperature. If we were able to cool the system to a lower temperature, amount of heat available for steam generation would be more. This results in an increase in power production, which could account for better efficiency at lower temperatures. However, the two main reasons for choosing 1,800°F as operating temperature are:

1. If we allow the combustion reaction to take place without a control in the temperature, it would reach around 3,600°F. Designing reactors that could handle that very high temperature would be expensive.
2. After wide sensitivity analysis, 1,800°F was found to be a feasible temperature within the range cited in literature and also to result in lower nitrogen oxide emissions.

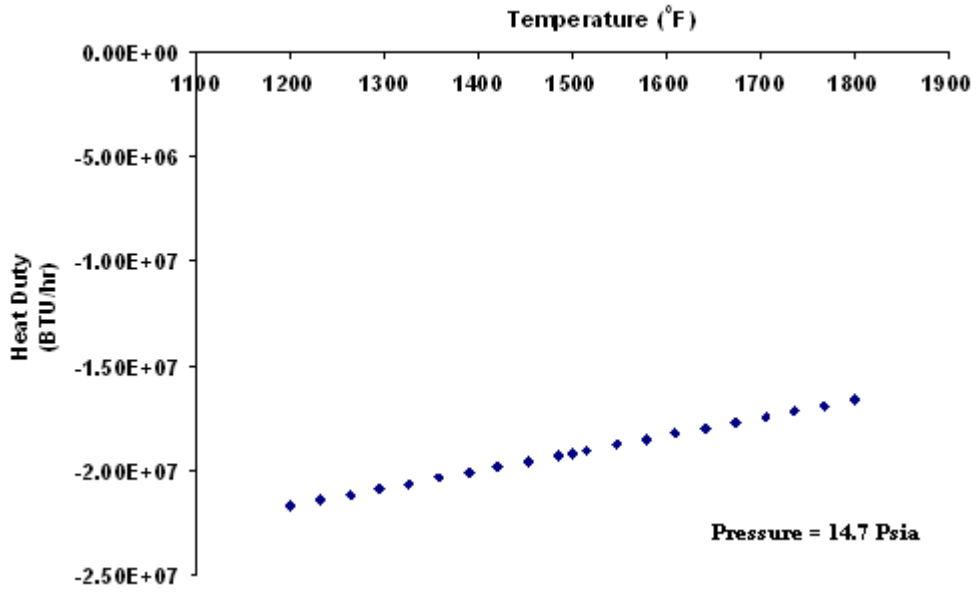

Fig. 5.11 - Heat duty variation with combustion temperature

5.3 Atmospheric Emissions

Atmospheric emissions are of significant concern in both the combustion and the gasification process. We analyzed emission of the gaseous pollutants like SO_x, NO_x, and CO_2. Particulate emissions are also addressed in this section. Table 5.1 shows the

emission of pollutant gases and particulate matter in both gasification and combustion processes.

Table 5.1 Emission of pollutants in the combustion and gasification process

Pollutant	Mass Flow Rate (lb/hr)		Flow Rate (in lb/MMBTU)	
	Combustion	Gasification	Combustion	Gasification
SO_2	---	0.2813	---	$2.17x10^{-2}$
NOx	2.27	0.0088	0.263	$6.76x10^{-4}$
CO_2	6902	6896	798.8	514.35
Ash Removed	10.6	10.6	---	---
Ash Remaining	0.00	0.00	---	---
Sulfur (lb/hr feedstock)	---	0.0515	---	---
Calcium Sulfate (lb/hr feedstock)	0.227	---	---	--

5.3.1 SO_2 Emissions

The gas turbine in the gasification process is intolerant to H_2S (hydrogen sulfide). Hence, H_2S is mostly removed in the acid gas removal unit and sent to the Claus process before the syngas enters the gas turbine for further combustion. The sulfur present in the syngas is removed as elemental sulfur. Only trace sulfur dioxide in the syngas is formed by the combustion process in the gas turbine. The emission from the combustion process is very small because SO_x reacts with limestone to form to calcium sulfate, and 2,135 lb/hr of petcoke feedstock results in the formation of 485 lb/hr of calcium sulfate. For the gasification process, about 110 lb/hr of elemental sulfur is recovered for the same amount of feedstock. SO_2 formed as a result of combustion in the gas turbine is 2.17×10^{-2} lb / MMBTU.

5.3.2 NO_x Emissions

We also modeled NO_x emissions ($NO_x = NO + NO_2$) in the study. NO_x coming out of the combustion process is higher than the NO_x that evolves from the gasification process. In the gasification, NO_x mainly forms during combustion process in the gas turbine combustor. The NO_x that evolves from combustion is 0.26 lb/MMBTU, compared to 6.8×10^{-4} lb/MMBTU that evolves from the gasification process. NO_x levels in the gasification process are below 550 ppm, which is the permissible emission limit level established in the industry for this type of facility. Table 5.2 shows the emission limit specified in United States.[28]

Table 5.2: US clear skies emission limits of the pollutants

Pollution	Emission Limit (lb/MWh)
Sulfur dioxide (SO_2)	2.00
Nitrogen Oxide (NO)	1.00
Carbon dioxide (CO_2)	0.20

5.3.3 CO_2 Emissions

Both processes produce CO_2 emissions. Because the gasification process is more energy efficient, it produces less CO_2. In the combustion process, CO_2 is the main component in the flue gas, and only minimal amounts of CO evolve. In the gasification process, syngas CO is converted to CO_2 by combustion in the gas turbine section. CO emissions from the gas turbines are below 5 ppm, so a conversion of nearly 100% is

assumed. From Fig. 5.12, we observe that the amount of CO_2 in the combustion process is 2.78 lb/kWh, compared to the gasification process at 1.81 lb/kWh.

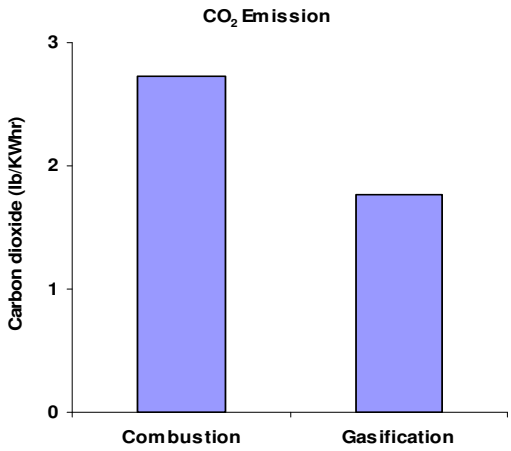

Fig. 5.12 - Carbon dioxide emission comparison in both the processes

5.3.4 Particulate Emissions

Solids like ash, particulate matter, and traces of metal present in the feedstock material come out as a residue. Disposal of this solid refuse is a challenging task. If these solids contain toxic materials like heavy metals, they should be disposed safely. Landfill is the usual disposal technique for these materials. We modeled solids emissions removal with a gas cyclone separator. Compared to bag house filters, cyclones have a wide operating temperature range. For combustion, solids emissions removal depends on the type of combustor used and can reach efficiency up to 100%. In gasification, two units are used for solids removal, a cyclone that removes the gross ashes and attains 98% efficiency and a venturi scrubber that reduces the total solids to 2.17 ppm in mass. The

acid gas removal unit contains filters[6] that retain the rest of the solids required for achieving a particle matter concentration lower than 0.005, which is the gas turbine specification.

5.3.5 Sulfur Removal

Sulfur is removed in its elemental form in the gasification process by a Claus process. The amount of sulfur generated in the gasification process is 110 lb/hr of Sulfur per 2135 lb/hr of feedstock. The Claus processes greatly helps in converting sulfur-bearing syngas to elemental sulfur, thereby reducing the sulfur dioxide in the flue gas coming out of the gas turbine after the syngas combustion process. For combustion, sulfur dioxide in the flue gas is converted to calcium sulfate by treatment with limestone, obtaining 485 lb/hr of calcium sulfate per 2,135 lb/hr of feedstock.

5.4 Power Consumption and Generation by the Utilities in the Combustion Process

Overall power generated by the process units and utilities load in the combustion model is given in the Table 5.3.

Table 5.3 – Power generated and utilities load in the combustion process

Process	Power Generated / Load (MW)
Power Generated (Heat and Shaft Power)	
Combustor	5.40
High-pressure Steam Turbine	2.38
Low-pressure Steam Turbine	0.52
Total Available Power	**+8.30**
Major Utilities Power Load	
Crushing	-0.0049
Bag Filter	-0.0001
Calcinizer	-0.0532
Heat Exchanger	-5.15
Pump 1	-0.163
Pump 2	-0.022
Pump 3	-0.0027
Sulfur Separator	-0.0002
Total Utilities Load	**-5.39**
Overall Power Generated	**+2.91**

5.5 Power Consumption and Generation by the Utilities in the Gasification Process

Overall power generated by the process units and utilities load in the gasification model is given in the Table 5.4.

Table 5.4 Power generated and utilities load in the gasification process

Process	Power Generated / Load (MW)
Power Generated	
Gas Turbines	6.42
Steam Turbines	1.02
Cooling Section	0.18
Total Available Power	**+7.62**
Major Utilities Power Load	
Crusher	-0.0049
Heater	-0.14
Claus Process	-0.273
Gas Compressors	-1.80
HRSG Section	-1.51
Total Utilities Load	**-3.73**
Overall Power Generated	**+3.89**

5.6 Overall Efficiency of Combustion and Gasification

Overall plant efficiencies for combustion and gasification are explained in this section.

5.6.1 Efficiency of Combustion Process

Overall efficiency is calculated using the following formula:

$$\eta_{Overall} = (W_{NE} \times 3600 \times OH) / (\dot{m}_{Petcoke} \times LHV_{Petcoke}) \quad (36)$$

Where $\eta_{overall}$ is the overall plant efficiency, W_{NE} is the total energy generated by the plant, OH is the total operating hours available in a year, $\dot{m}_{Petcoke}$ is the mass flow rate of petcoke, and $LHV_{Petcoke}$ is the lower heating value of petcoke. Substituting, the assumption of 300 days of plant availability, we get:

$$\dot{m}_{Petcoke} = 2135 \text{ lb/hr} = 2135 \times 24 \times 300 \times 0.00045359$$

$$= 6972 \text{ tons/yr}$$

LHV of petcoke is calculated using Chaniwalah-Parikh correlation,[2]

$$HHV \text{ (MJ/kg)} = 34.91C + 117.83H - 10.34O - 1.51N + `10.05S - 2.11Ash \quad (37)$$

Using obtained HHV corresponding LHV is computed for the petcoke.

$$\eta_{Overall} = (2.91 \times 3600 \times 24 \times 300 \times 100) / (6972 \times 35424) = 30.54$$

5.6.2 Efficiency of Gasification Process

Overall efficiency is calculated using Eq. 36.

Substituting the assumption of 300 days of plant availability, we get:

$$\eta_{Overall} = (3.89 \times 3600 \times 24 \times 300 \times 100) / (6972 \times 35424) = 40.82$$

6. ECONOMIC ANALYSIS OF THE PROCESSES

Plant economics play an important role in deciding whether the process is efficient or not. This section explains the capital expenditures for commissioning unit operations of gasification and combustion processes.

6.1 Capital Cost for Gasification Process

The gasification process involves many unit operations. Capital expenditures were calculated using the correlations deduced by Caputo et al.[29, 30] Total capital expenditures are estimated as USD 7.09 million for a 3.89 MW power plant. Normalized capital cost is found to be 1,857 USD/kW. Table 6.1 shows the important correlations used for calculating capital expenditures of certain unit operations.

Table 6.1 Correlations used for calculating CapEx of gasification process

Unit Operation	Correlations Used (in $)
Pump	$28000(N_{ST})^{0.5575} \times 1.41$
Compressor	$11400(N_{TE})^{0.5575} \times 1.41$
Gasifier	$1600(M_{G/CC})^{0.917} \times 1.41$
Heat Exchanger	$51500(N_{ST})^{0.5129} \times 1.41$
Sulfur removal	$126000(N_{TE})^{0.5885} \times 1.41$
Particulate Separator	$93500(N_{TE})^{0.4425} \times 1.41$
Steam Turbine	$633000(N_{ST})^{0.398} \times 1.41$
Gas Turbines	$3800(N_{GT})^{0.754} \times 1.41$
Condenser	$398000(N_{ST})^{0.333} \times 1.41$
Auxiliary Services	0.1 x TCI

N_{ST} = Power generated by steam cycle (in MW)

N_{GT} = Power generated by gas turbine cycle (in MW)

N_{TE} = Power generated by both steam cycle and gas turbine cycle (in MW)

$M_{G/CC}$ = Flow rate of petcoke (kg/hr)

TCI = Total Capital Investment (in $)

6.2 Operating Cost for Gasification Process

Operating expenses in a process industry are generally high. They are the main driving force to determine the margin of profit for any given fiscal year. Operating expenses for the gasification plant are divided into 6 divisions. Cost was allocated to each division based on a model given by Caputo et al. [29] The main equations used for calculating the operating expenses are shown in Table 6.2.

Table 6.2 Correlations used for calculating OpEx of gasification process

Operating Expenses	Correlations Used (in $)
Ash Transportation Cost	$62(M_A)\times 1.41$
Ash Disposal Cost	$24(M_A)\times 1.41$
Personnel Cost	$26000(n_p)\times 1.41$
Feedstock Cost	$0.75(M_F)$
Maintenance Cost	0.03 x TCI
Insurance and General	0.01 x TCI

M_A = Flow rate of Ash (in kg/hr)

M_F = Flow rate of petcoke in terms of energy (in MMBTU/yr)

n_P = Number of personnel working in the plant

TCI = Total Capital Investment (in $)

6.3 Cash Flow for Gasification Process

Power price is highly dependent on availability and demand. We took the average power as 7.82 cents/kW. The total revenue is found to be, USD 2.1 million/year for the plant considered. Payback depends on the profit margin of the gasification process. Profit is determined by deducting the operating expenses from the revenue. For the plant we modeled, profit is found to be, USD 0.58 million/year. The payback period for our gasification plant model is 12.1 years.

6.4 Capital Cost for Combustion Process

Combustion process involves many unit operations. Capital expenditures were calculated using the correlations deduced by A.C. Caputo et al. Total capital expenditures are estimated as USD 2.31 million for a 2.91 MW power plant. Normalized capital cost is found to be 915 USD/kW. Table 6.3 shows the important correlations used for calculating capital expenditures of certain unit operations.

Table 6.3 Correlations used for calculating CapEx of combustion process

Unit Operation	Correlations Used (in $)
Pump	$28000(N_{TE})^{0.5575} \times 1.41$
Compressor	$11400(N_{TE})^{0.5575} \times 1.41$
Combustor	$134000(N_{TE})^{0.694} \times 1.41$
Heat Exchanger	$51500(N_{TE})^{0.5129} \times 1.41$
Calcinizer	$126000(N_{TE})^{0.5885} \times 1.41$
Particulate Separator	$93500(N_{TE})^{0.4425} \times 1.41$
Steam Turbine	$633000(N_{TE})^{0.398} \times 1.41$

N_{TE} = Power generated in combustion process (in MW)

6.5 Operating Cost for Combustion Process

Similar to the gasification process, operating expenses for the combustion plant are divided into 6 divisions. Cost was allocated to each division based on a model given by Caputo et al. The main equations used for calculating the operating expenses are shown in Table 6.4.

Table 6.4 Correlations used for calculating OpEx of combustion process

Operating Expenses	Correlations Used (in $)
Ash Transportation Cost	$62(M_A)\times 1.41$
Ash Disposal Cost	$24(M_A)\times 1.41$
Personnel Cost	$26000(n_p)\times 1.41$
Feedstock Cost	$0.75(M_F)$
Maintenance Cost	0.03 x TCI
Insurance and General	0.01 x TCI

M_A = Flow rate of Ash (in kg/hr)

M_F = Flow rate of petcoke in terms of energy (in MMBTU/yr)

n_P = Number of personnel working in combustion plant

TCI = Total Capital Investment of combustion plant (in $)

6.6 Cash Flow for Combustion Process

Similar to gasification, the power price is taken as 7.82 cents /kW. The total revenue is found to be USD 1.42 million/year for the plant considered. Payback depends on the profit margin of the gasification process. Profit is determined by deducting the operating expenses from the revenue. For the plant, profit is USD 0.243 million/year. The payback period for the designed combustion plant model is 9.5 years.

6.7 Comparison of Cost Analyses for Both Processes

From Tables 6.1 to 6.4, we can infer that total payback time for the combustion process is half that of the gasification process. Fig. 6.1 shows the payback period of both combustion and gasification processes. Total power that will be generated by the gasification model is 3.89 MW for 2135 lbm of petcoke whereas for combustion it is 2.91 MW. We can deduce that capital cost is 1,857 USD/kW for gasification and that of combustion is 915 USD/kW. The values are competitive for both the models, considering that emission is curtailed very much than those cited in the literature. Fig. 6.2 shows the breakeven cost of the two processes. Combustion payback may be low compared to the gasification because combustion has fewer unit operations. The profits from the gasification process break even with combustion at around 14 yrs. Fig. 6.3 shows the capital cost share for each process section for gasification, and Fig. 6.4 shows the capital cost share for each process section of the combustion process. From the diagram we can see that the major share of capital expenditure goes for the steam turbine section in a gasification process. For a combustion process, the major share goes to the steam turbine section and the combustion section.

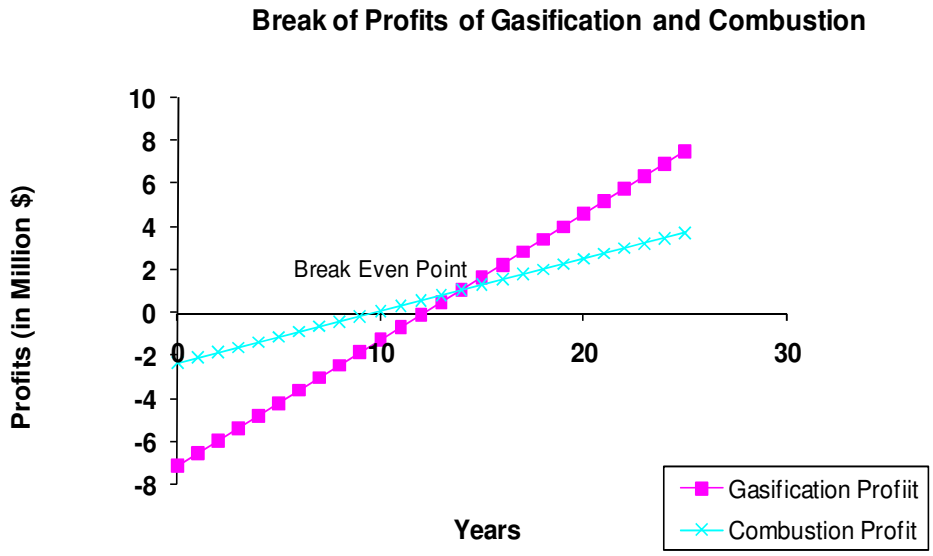

Fig. 6.1 - Profit breakeven for combustion and gasification

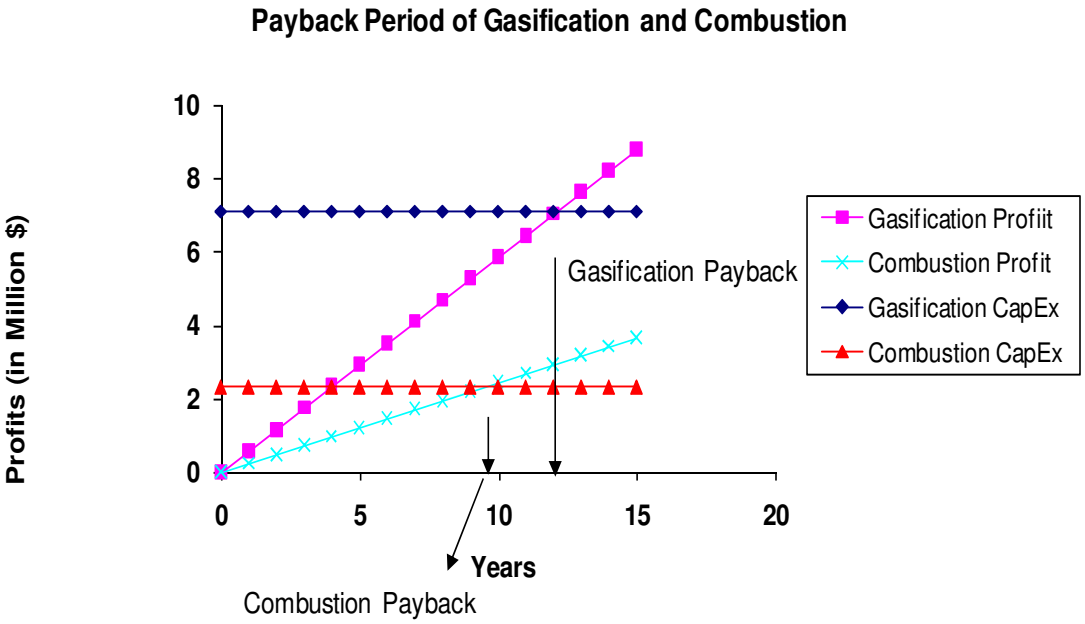

Fig. 6.2 - Payback period for combustion and gasification

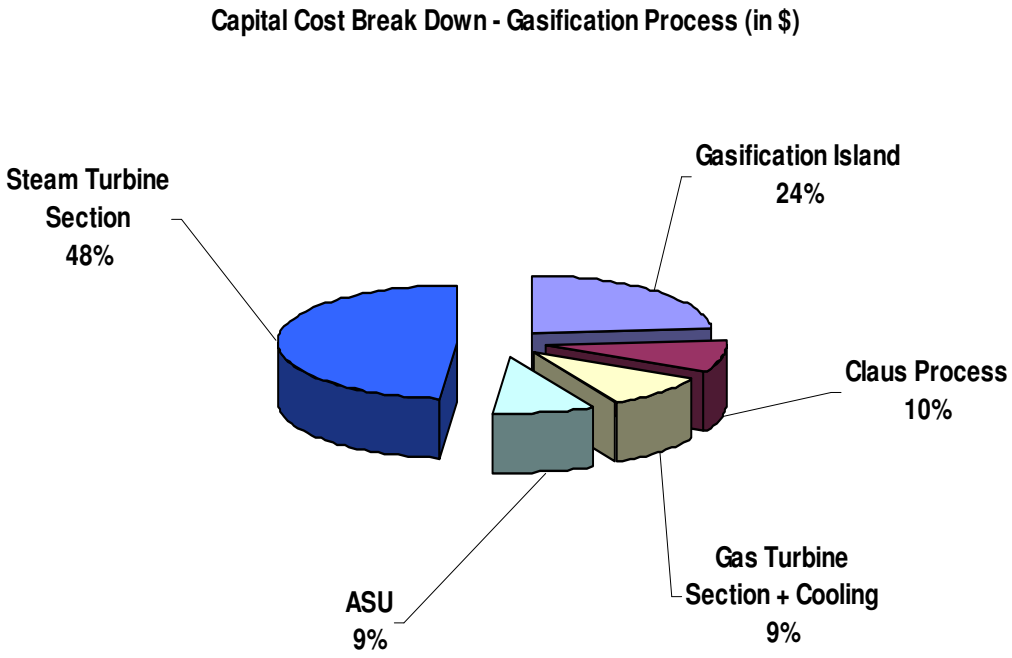

Fig. 6.3 - Capital cost distribution for the gasification process

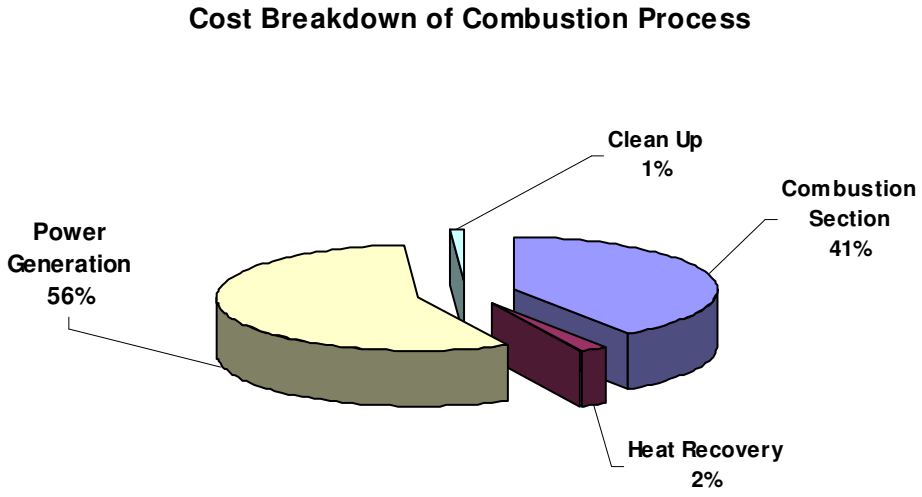

Fig. 6.4 – Capital cost distribution for the combustion process

The main assumptions used in calculating the revenue and profit are given in Table 6.5.

Table 6.5 - Assumptions used in cost analysis [31, 32]

Parameter	Assumption
Availability of Plant	300 Days/yr
Electricity Cost	7.82 cents / kW
Sulfur Cost	1$ / 1 lb
Number of Personnel for Gasification Plant	30
Number of Personnel for Combustion Plant	20
1 Euro	1.41 Dollars

Since total sulfur produced in the model is negligible, we neglected the cost that it could add to the revenue. For a large-scale gasification process, sulfur is valuable by product.

7. CONCLUSIONS AND RECOMMENDATIONS

7.1 Conclusions

Process models of both processes were carried out with Tuscaloosa petcoke feedstock composition, which is typical for refineries on the coast of the Gulf of Mexico. Modeling results indicate that for 2135 lbm / hr of petcoke, combustion will generate about 2.91 MW and gasification will generate 3.89 MW of net available power. Optimal overall efficiency of the gasification process is computed as 41%, and for the combustion process it is computed as 31%. Optimum values of process variables are shown in Table 7.1.

Table 7.1 – Optimum process parameter values for both processes

Combustion		Gasification	
Temperature (^{o}F)	1800	Temperature (^{o}F)	2552
Pressure (psia)	14.7	Pressure (psia)	650
Steam (lbmol / lbm of Petcoke)	---	Steam (lbmol / lbm of Petcoke)	0.017
Air (% Stoichiometric air required)	102	Oxygen (lbmol / lbm of Petcoke)	0.028

Cost analysis shows that gasification has an upper edge over combustion, despite its high capital expenditure. Both processes have a rate of return greater than 30% with certain assumptions such as operating hours, petcoke composition used, personnel required, and plant facilities. Combustion and gasification processes break even at around 14 yrs after the initial production. This breakeven solely depends on the profits, which in turn are affected by major factors like gas price, demand, and supply. Even though petcoke exports have increased over the period of years shown in Fig. 1.1, industries in US can consider using available petcoke instead of exporting it to meet their power needs by adopting either of the two processes, depending on the requirements.

7.2 Recommendations for Future Work

The following additional study should be considered:

1. A deterministic approach to model the process in Aspen using the kinetics.
2. Other methods to improve the efficiency of the processes without increasing emissions. Thermal efficiency greatly influences the amount of power generated.
3. A probabilistic approach to determine the cash flow for cost economics. This would give a more information on the payback and downside risk.

NOMENCLATURE

W_{pump} = work done by pump shaft, MW

$W_{turbine}$ = work done by turbine shaft, MW

Q_{in} = heat supplied to unit operation, MMBTU/hr

Q_{out} = heat rejected from the unit operation, MMBTU/hr

$\dot{m}$ = steam mass flow rate, lb/hr

h_i = mass enthalpy of stream i, BTU/lb

η = thermal efficiency of cycle, %

$M_{G/CC}$ = Flow rate of petcoke, kg/hr

M_A = Flow rate of Ash, kg/hr

M_F = Flow rate of petcoke in terms of energy, MMBTU/yr

N_{ST} = power generated by steam cycle, MW

N_{GT} = power generated by gas turbine cycle, MW

N_{TE} = power generated by both steam cycle and gas turbine cycle, MW

n_P = number of personnel working in combustion plant

ν = volume of fluid entering the unit operation block, ft^3/hr

p = pressure, psia

W = work done by the unit operation, MW

η = efficiency of the unit operation block

H_i = overall enthalpy of the stream i, MMBTU/hr

U_i = internal energy of the stream i, MMBTU/hr

E_{in} = overall energy of the inlet stream, MMBTU/hr

E_{out} = overall energy of the outlet stream, MMBTU/hr

v = velocity of the stream i, ft/s

g = acceleration due to gravity, ft^2/s

z = datum height, ft

h_R = heat of reaction,

N_i = number of moles of the stream i

$\bar{h}_f^{\,o}$ = heat of formation of the component, kJ/kmol

$\bar{h}^{\,o}$ = sensible enthalpy of the component at 298 K and 1 atm, kJ/kmol

γ = compression ratio of inlet to outlet pressure

R = universal gas constant, kJ/kmol K

T_i = temperature of the stream i, ^oF

c_p = specific heat at constant pressure, kJ/kmol K

c_v = specific heat at constant volume, kJ/kmol K

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APPENDIX

Sample energy balance calculations around various unit operations

Gasification Island

Work done by the pump

The pump used here is for increasing the pressure of the water to be converted into steam.

The volume of water entering the pump and leaving pump remains constant.

Volume of water entering (v) = 10.16 ft^3/hr

Volume of water entering and leaving remains the same.

The pressure changes between the inlet and outlet pressures are:

Pressure change in pump (dp) = 420.4 psia.

Work done given by the pump is given by the equation:

$$W = \Delta(pv) = v(dp) \qquad \text{(A -1)}$$

Work done by the pump (W_{ideal}) = 830.62 kJ/hr

= 0.000,8 MMBTU/hr

So with 90% efficiency of pump, work done = $\frac{W_{ideal}}{\eta_{pump}}$ (A-2)

So total work done at 90% efficiency is $= \frac{0.000,8}{0.9} = 0.000,9 \text{MMBTU / hr}$

Total energy balance around the pump is given by: $H = U + V\,dp$ (A-3)

Enthalpies of inlet and outlet stream associated with the unit operation process are shown in the Fig. A-1.

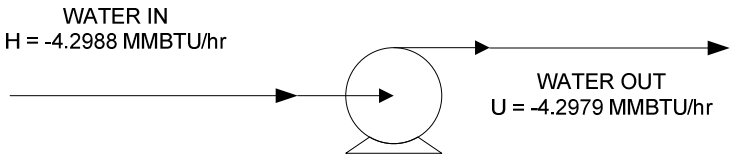


Fig. A-1 - Energy balance around pump.

Work done by the pump using the Eq. A-1is:

$$V\,dp = H - U = 0.000{,}9\ \text{MMBTU/hr}$$

Work done above is same as the value obtained from calculation.

Fig. A-2 shows the results of the unit operation with Mass and energy balance around the unit operation.

Pump results

Fluid power:	0.00023178	MW
Brake power:	0.00025194	MW
Electricity:	0.25194493	kW
Volumetric flow rate:	10.1661314	cuft/hr
Pressure change:	420.413213	psi
NPSH available:	33.0615525	ft-lbf/lb
NPSH required:		
Head developed:	976.080183	ft-lbf/lb
Pump efficiency used:	0.92	
Net work required:	0.33786371	hp

Mass and energy balance

Total		In	Out	Rel. diff
Mole-flow:	lbmol/hr	35	35	0
Mass-flow:	lb/hr	630.5348	630.5348	0
Enthalpy:	Btu/hr	-4298761.9	-4297902.2	-0.0001999

Fig. A-2 Mass and energy balance results around pump

Energy Balance around Compressor:

Compressor is used to compress the oxygen to be fed into the gasifier to certain higher pressure.

Inlet Pressure of Oxygen Stream Entering Compressor = 14.7 psia

Outlet Pressure of Oxygen coming out of Compressor = 609.15 psia

R/cP value from Aspen $(\gamma - 1)/\gamma = 0.28$

Ratio of Outlet to Inlet Pressure $P_2/P_1 = 41.44$

Inlet Temperature of Oxygen Stream $T_{in} = 298.15$ K

Outlet Temperature of Oxygen Stream coming out of compressor is calculated by:

$$T_{out} = T_{in}\,(P2/P1)^{(\gamma-1)/\gamma} \qquad \text{(A-4)}$$

Calculated value of T_{out} = 1081 F

Simulated value of T_{out} from Aspen = 1066 F

Molecular weight of the oxygen stream = 31.79 kg/kmol

So R in terms of (kJ/kg K) is given as = R (in kJ/kmol K) / Molecular Weight

$$= \frac{8.314}{31.79} = 0.26 \text{ kJ/kg K}$$

Work done by the Compressor (Win) is given by the following equation.

$$W_{comp,\,in} = \frac{\gamma R T_{in}}{\gamma - 1}\left(\left(\frac{P_{out}}{P_{in}}\right)^{\left(\frac{\gamma-1}{\gamma}\right)} - 1\right) \qquad \text{(A-5)}$$

Using the above equation calculating the value of $W_{comp,in}$ = 515.27 kJ/kg

Mass of Oxygen entered into the compressor = (m) = 869.36 kg/hr

$$\text{So, Wcomp,in in kJ/hr} = \text{Mass of Oxygen Entered (in kg/hr)} \times \text{Work (in kJ/kg)}$$

$$= 515.27 \times 869.36 = 447961.45 \text{ kJ/hr} = 424585.52 \text{ BTU/hr}$$

But the above calculated work done is for 100% efficient compressor. So Work input for a 92% efficient compressor is given by:

$$\frac{\text{Work done at 100\% efficiency}}{\text{Percentage Efficiency}}$$

So final work input for the compressor is = $\frac{424585.52}{0.92} = 461506\ \text{BTU/hr}$

= 0.4615 MMBTU/hr

Overall Enthalpy balance around compressor is given as:

$$\text{Energy In} = \text{Energy Out}$$

which is given by the following equations:

$$E_{out} = Q_{out} + \dot{m}H_2 + (\frac{\dot{m}v^2}{2}) + \dot{m}gz_2 \qquad \text{(A-6)}$$

$$E_{in} = W_{in} + \dot{m}H_1 + (\frac{\dot{m}v^2}{2}) + \dot{m}gz_1 \qquad \text{(A-7)}$$

Neglecting the potential and kinetic energy effects we can calculate the final heat out from the compressor (Q_{out})

$$\text{So from the Balance } Q_{out} = W_{comp,in} + H_{in} - H_{out} \qquad \text{(A-8)}$$

Where H_{in} from Aspen is = -1.43E-09 MMBTU/hr

H_{out} from Aspen is = 0.451 MMBTU/hr

So Q_{out} = 0.4615 -1.43E-09 - 0.451 = 0.00106 MMBTU/hr

Fig. A-3 shows the results of the unit operation with Mass and energy balance around the unit operation.

Compr results

Compressor model:	Isentropic Compressor	
Phase calculations:	Vapor phase calculation	
Indicated horsepower:	0.13215489	MW
Brake horsepower:	0.13215489	MW
Net work required:	0.13215489	MW
Power loss:	0	hp
Efficiency:	0.92	
Mechanical efficiency:	1	
Outlet pressure:	609.158498	psi
Outlet temperature:	1066.19785	F
Isentropic outlet temperature:	992.045131	F
Vapor fraction:	1	
Displacement:		
Volumetric efficiency:		

Mass and energy balance

Total		In	Out	Rel. diff
Mole-flow:	lbmol/hr	60.2717	60.2717	0
Mass-flow:	lb/hr	1916.61197	1916.61197	0
Enthalpy:	MW	-4.188E-10	0.1321549	-1

Fig. A-3 Mass and energy balance results around compressor

Energy Balance around Gasifier:

Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the Fig. A-4.

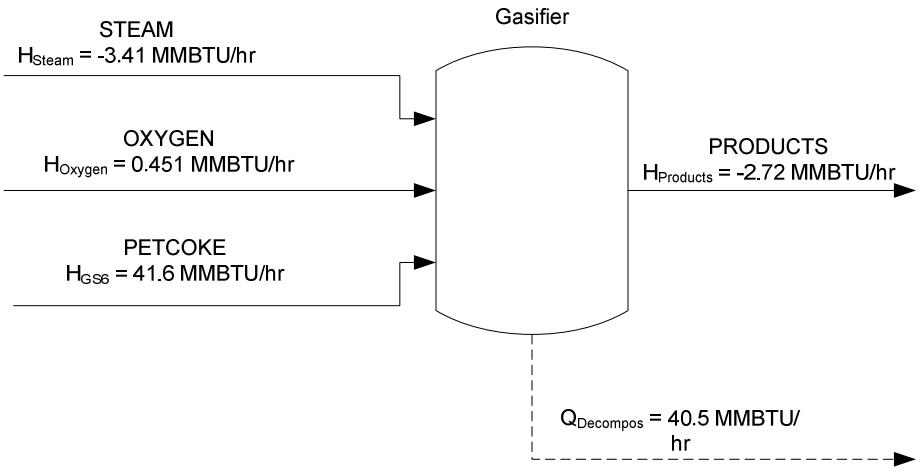


Fig. A-4 Energy balance around gasifier

Overall Energy In into the gasifier is given by the following equation:

$$E_{in,gasifier} = \Sigma H_{reactants} - Q_{decompos} \qquad \text{(A-9)}$$

So overall energy in the Gasifier is $E_{in,gasifier} = H_{steam} + H_{oxygen} + H_{Petcoke} - Q_{decompos}$

= -1.79 MMBTU/hr

Enthalpy of outlet stream (products) from Gasifier = *(from Aspen)*

= -2.72E+00 MMBTU/hr

So the overall heat duty of the gasifier is given by the following equation:

$$Q_{in} + \sum h_{reac} - \sum h_{prod} = 0 \qquad \text{(A-10)}$$

So heat duty of the gasifier ($Q_{in,gasifier}$) = -2.72 + 1.79 = 0.93 MMBTU/hr (Calculated)

Heat duty of Gasifier value from Aspen = 0.93 MMBTU/hr

So both the heat duties i.e., calculated and simulated values are equal and this verifies the energy balance around gasifier and gasification island.

Fig. A-5 shows the results of the unit operation with Mass and energy balance around the unit operation.

RGibbs results

Outlet temperature:	2552	F
Outlet pressure:	650	psi
Heat duty:	-12.134923	MW
Net heat duty:	-12.134923	MW
Vapor fraction:	1	
Number of fluid phases:	1	
Maximum number of pure solids:	0	

Mass and energy balance

Total		In	Out	Generated	Rel. diff
Mole-flow:	lbmol/hr	301.404879	238.10631	-63.298569	-9.43E-17
Mass-flow:	lb/hr	4682.10335	4682.10335		4.2735E-15
Enthalpy:	MW	11.3379868	-0.7969364		1.07028906
Conventional components					
Mole-flow:	lbmol/hr	301.404879	238.10631	-63.298569	-9.43E-17
Mass-flow:	lb/hr	4671.51338	4671.51338		4.2832E-15
Non-conventional components					
Mass-flow:	lb/hr	10.5899674	10.5899674		0

Fig. A-5 Mass and energy balance results around gasifier

Cooling

Cooling section has three coolers which bring down the temperature of hot syngas coming out of the gasifier. This is done mainly to reduce the temperature of the syngas before it enters the gas cleanup process.

Energy Balance around COOLER1:

Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the Fig. A-6.

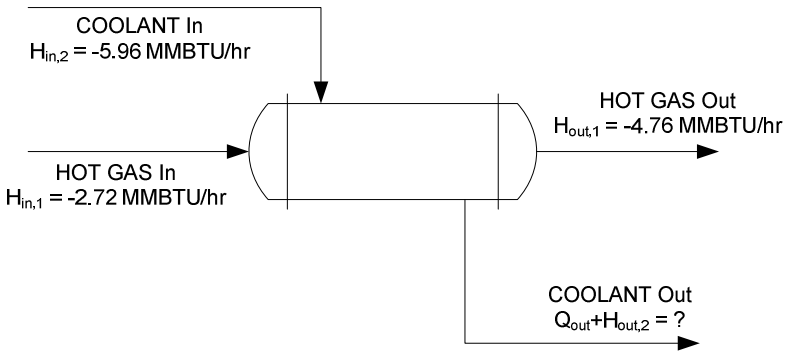


Fig. A-6 Energy balance around cooler1

Overall Energy balance around the Cooler is given by the following equations:

$$\text{EnergyBalance} = E_{in} - E_{out} = 0 \qquad \text{(A-11)}$$

$$E_{in} = W_{in} + Q_{in} + \sum H_{in} \qquad \text{(A-12)}$$

$$E_{out} = W_{out} + Q_{out} + H_{out} \qquad \text{(A-13)}$$

In a cooler Work is not done. So $W_{in} = W_{out} =$ 0 MMBTU/hr

Similarly no heat is supplied into the cooler. So $Q_{in} =$ 0 MMBTU/hr

So by the energy balance we have

$$H_{2,out} + Q_{out} = \Sigma H_{in} - H_{1,out} \qquad \text{(A-14)}$$

So $H_{2,out}+Q_{out}$ is calculated as = -3.92 MMBTU/hr

Q_{out} is the amount of heat rejected in this cooling process. By this way of cooling the temperature of the syngas is reduced from 2,550 F to 1,500 F. The steam generated by this cooling process is rerouted to HRSG, where all the steam streams are coupled to generate steam for steam turbine section

Fig. A-7 shows the results of the unit operation with Mass and energy balance around the unit operation.

Heatx results

	Inlet		Outlet	
Hot stream:	PRODUCTS		COOLGAS1	
Temperature:	2552	F	1500	F
Pressure:	650	psi	650	psi
Vapor fraction:	1		1	
Cold stream:	COOLH2O1		H2OST1	
Temperature:	77	F	1105.96062	F
Pressure:	14.7	psi	14.7	psi
Vapor fraction:	0		1	
Heat duty:	0.5986867	MW		

Mass and energy balance

Total		In	Out	Rel. diff
Mole-flow:	lbmol/hr	311.654987	311.654987	0
Mass-flow:	lb/hr	6007.10335	6007.10335	0
Enthalpy:	MW	-3.4443585	-3.4443585	8.8929E-09
Conventional components				
Mole-flow:	lbmol/hr	311.654987	311.654987	0
Mass-flow:	lb/hr	5996.51338	5996.51338	0
Non-conventional components				
Mass-flow:	lb/hr	10.5899674	10.5899674	0

Fig. A-7 Mass and energy balance results around cooler1

Energy Balance around COOLER2:

Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the Fig. A-8.

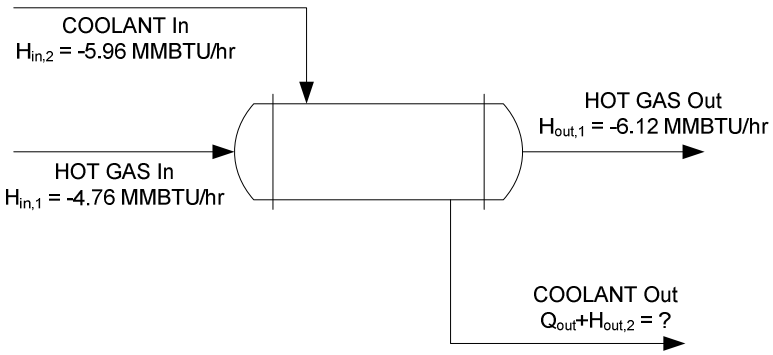


Fig. A-8 Energy balance around cooler2

Overall Energy balance around the Cooler is given by Eqs. A-11, A12, and A-13:

In a cooler Work is not done. So $W_{in} = W_{out} =$ 0 MMBTU/hr

Similarly no heat is supplied into the cooler. So $Q_{in} =$ 0 MMBTU/hr

So by Eq. A-14, we have:

So $H_{2,out}+Q_{out}$ is calculated as = -4.60 MMBTU/hr

Q_{out} is the amount of heat rejected in this cooling process in the steam. By this way of cooling the temperature of the syngas is reduced from 1,500 F to 750 F. The steam generated by this cooling process is rerouted to HRSG, where all the steam streams are coupled to generate steam for steam turbine section
Fig. A-9 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

Heatx results

	Inlet		Outlet	
Hot stream:	COOLGAS1		COOLGAS2	
Temperature:	1500	F	750	F
Pressure:	650	psi	650	psi
Vapor fraction:	1		1	
Cold stream:	COOLH2O2		H2OST2	
Temperature:	77	F	955.150571	F
Pressure:	14.7	psi	14.7	psi
Vapor fraction:	0		1	
Heat duty:	0.39784728	MW		

Mass and energy balance

Total		In	Out	Rel. diff
Mole-flow:	lbmol/hr	289.590384	289.590384	0
Mass-flow:	lb/hr	5609.60335	5609.60335	0
Enthalpy:	MW	-3.2488186	-3.2488186	2.3204E-09
Conventional components				
Mole-flow:	lbmol/hr	289.590384	289.590384	0
Mass-flow:	lb/hr	5599.01338	5599.01338	0
Non-conventional components				
Mass-flow:	lb/hr	10.5899674	10.5899674	0

Fig. A-9 Mass and energy balance results around cooler2

Energy Balance around COOLER3:
Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the Fig. A-10.

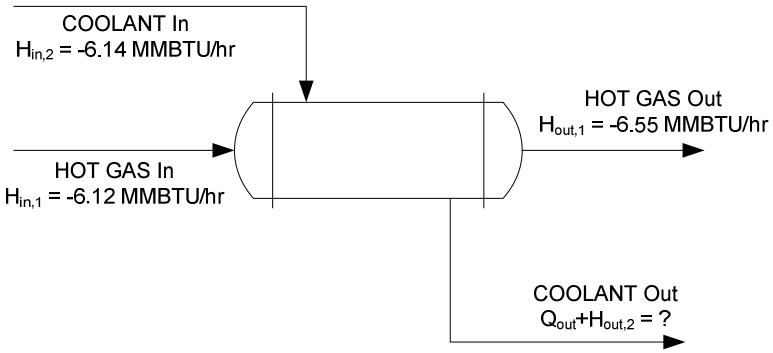


Fig. A-10 Energy balance around cooler3

Overall Energy balance around the Cooler is given by Eqs. A-11, A12, and A-13:

In a cooler Work is not done. So $W_{in} = W_{out}$ = 0 MMBTU/hr

Similarly no heat is supplied into the cooler. So Q_{in} = 0 MMBTU/hr

So by Eq. A-14, we have:

So $H_{2,out}+Q_{out}$ is calculated as = -5.17 MMBTU/hr

Q_{out} is the amount of heat rejected in this cooling process in the steam. By this way of cooling the temperature of the syngas is reduced from 750 F to 500 F. The steam generated by this cooling process is rerouted to HRSG, where all the steam streams are coupled to generate steam for steam turbine section

Fig. A-11 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

Heatx results

	Inlet		Outlet	
Hot stream:	COOLGAS2		COOLGAS3	
Temperature:	750	F	500	F
Pressure:	650	psi	650	psi
Vapor fraction:	1		1	
Cold stream:	COOLH2O3		H2OST3	
Temperature:	77	F	212.047553	F
Pressure:	14.7	psi	14.7	psi
Vapor fraction:	0		0.97539628	
Heat duty:	0.12621673	MW		

Mass and energy balance

Total		In	Out	Rel. diff
Mole-flow:	lbmol/hr	260.170913	260.170913	0
Mass-flow:	lb/hr	5079.60335	5079.60335	0
Enthalpy:	MW	-2.587697	-2.587697	6.5085E-09
Conventional components				
Mole-flow:	lbmol/hr	260.170913	260.170913	0
Mass-flow:	lb/hr	5069.01338	5069.01338	0
Non-conventional components				
Mass-flow:	lb/hr	10.5899674	10.5899674	0

Fig. A-11 Mass and energy balance results around cooler3

Gas Cleanup

Energy Balance around Selexol Process:

Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the Fig. A-12.

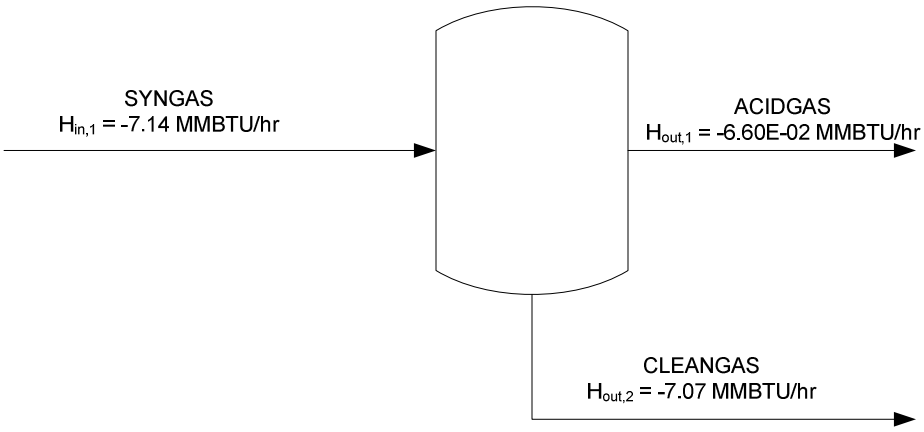


Fig. A-12 Energy balance around Selexol reactor

Selexol process is a separator to remove the acid gas from the syngas.

Total energy balance around the Selexol separator is given by the equation:

$$\text{Energy In} - \text{Energy Out} = 0$$

$$= -7.14 - (-6.60\text{E-}02 - 7.07) = 0 \text{ MMBTU/hr}$$

Fig. A-13 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

Mass and energy balance

	Total		In	Out	Rel. diff
	Mole-flow:	lbmol/hr	238.106276	238.106276	0
	Mass-flow:	lb/hr	4671.51236	4671.51236	1.9469E-16
▶	Enthalpy:	MW	-2.0911442	-2.0911443	4.0205E-08

Heat duty: -8.407E-08 MW

Split fractions in outlet streams

Substream: MIXED

Component ID	CLEANGAS	ACID-GAS
H2O	1	0
N2	1	0
O2	0	0
NO2	0	0
NO	1	0
S	0	1
SO2	0	1
SO3	0	0
H2	1	0
CL2	0	0
HCL	0	0
C	0	0
CO	1	0
CO2	0	1
H2S	0	1
CH4	0	0
COS	0	0
H3N	1	0
HCN	0	0
PETCOKE		
ASH		

Fig. A-13 Mass and energy balance results around Selexol reactor

Energy Balance around CFURNACE:

Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the Fig. A-14.

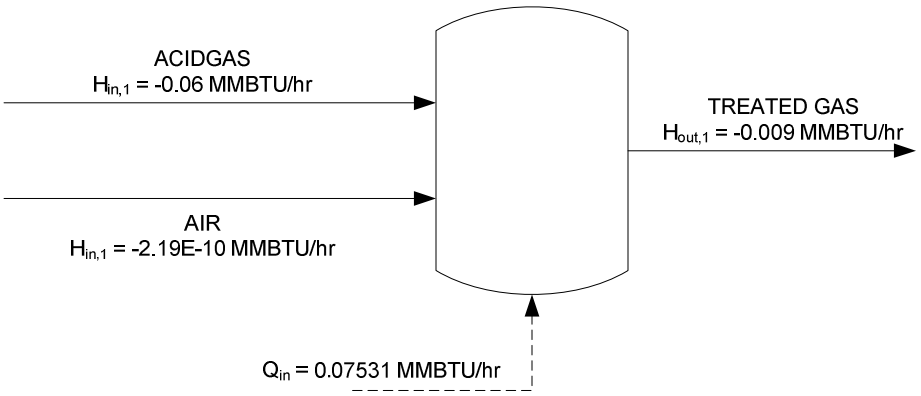


Fig. A-14 Energy balance around Claus furnace

According to the energy Balance overall energy balance around the furnace is given by the following equation:

$$\Sigma H_{in} - \Sigma H_{out} + Q_{in} = 0 \qquad \text{(A-15)}$$

So overall energy Balance is computed as : $- 0.066 - 2.19E - 10 + 0.075 + 0.0093 = 0$

We also need to compute the heat of reaction of the furnace. The two main reactions which take place in the reactor are:

$$H_2S + 1.5\,O_2 \text{ - - > } SO_2 + H_2O \qquad \text{(A - 16)}$$

$$2\,H_2S + SO_2 \text{ - - > } 2\,H_2O + 3S \qquad \text{(A - 17)}$$

The heat of reaction is given by the following equation:

$$h_R = \Sigma N_P (\bar{h}_f{}^o + \bar{h} - \bar{h}^o)_P - \Sigma N_R (\bar{h}_f{}^o + \bar{h} - \bar{h}_P{}^o)_R \qquad \text{(A-18)}$$

Where:

$\bar{h}_f{}^o$ is the heat of formation of the component

$\bar{h}^o$ is the sensible enthalpy of the component at 298 K and 1 atm

Sensible enthalpy is given by $c_P \times dT$

N is the number of moles of product or the reactants based on the stoichiometric reaction

The values of heat of formation, sensible enthalpy at furnace reactor conditions (i.e., at furnace temperature and pressure) and average enthalpy of each component from Aspen are given in tables A-1, A-2 and A-3.

Table A-1 Heat of formation values of components

Component Name	Chemical Formula	$\bar{h}_f^{\,o}$ value from Aspen (kJ/kmol)
Water	H_2O	-43874.83
Hydrogen Sulfide	H_2S	-6075.42
Oxygen	O_2	0.0000
Sulfur dioxide	SO_2	-22956.16
Sulfur	S	-10955.59

Table A-2 Sensible enthalpy values of components

Component Name	Chemical Formula	$\bar{h}^{\,o}$ value from Aspen (kJ/kmol)
Water	H_2O	45967.96
Hydrogen Sulfide	H_2S	10501.36
Oxygen	O_2	8684.35
Sulfur dioxide	SO_2	13202.65
Sulfur	S	7521.57

Table A-3 Average enthalpy values of components

Component Name	Chemical Formula	$\bar{h}$ value from Aspen (kJ/kmol)
Water	H_2O	-217850.00
Hydrogen Sulfide	H_2S	-118920.00
Oxygen	O_2	-27155.42
Sulfur dioxide	SO_2	-359980.00
Sulfur	S	229740.85

The extent of reaction 1 is assumed to be 40% conversion of the H_2S entering the system

So according to the stoichiometric reaction the heat of reaction for 1 kmol of H_2S entering the system, it is computed as:

$$h_{R1} = \Sigma N_{SO_2}(\bar{h}_f^{\,o} + \bar{h} - \bar{h}^{o})_{SO_2} + \Sigma N_{H_2O}(\bar{h}_f^{\,o} + \bar{h} - \bar{h}^{o})_{H_2O} - \Sigma N_{H_2S}(\bar{h}_f^{\,o} + \bar{h} - \bar{h}_P^{\,o})_{H_2S} - \Sigma N_{O_2}(\bar{h}_f^{\,o} + \bar{h} - \bar{h}_P^{\,o})_{O_2} \quad \text{(A-19)}$$

So computing the value of $h_{R1}(1kmol) = -514575.16$ kJ/kmol

Above is the value of heat of reaction for 1 kmol of H_2S.

For 0.9375 kmol of H_2S the heat of reaction is computed as:

$$= -514575.1635 \times 0.9375 \text{ kJ/kmol} = -482447.08 \text{ kJ/kmol}$$

Similarly we can compute heat of reaction for the reaction 2 using the following equation:

$$h_{R2} = \Sigma N_S (\bar{h}_f^{\,o} + \bar{h} - \bar{h}^{o})_S + \Sigma N_{H_2O} (\bar{h}_f^{\,o} + \bar{h} - \bar{h}^{o})_{H_2O} - \Sigma N_{H_2S} (\bar{h}_f^{\,o} + \bar{h} - \bar{h}_P^{\,o})_{H_2S} - \Sigma N_{SO_2} (\bar{h}_f^{\,o} + \bar{h} - \bar{h}_P^{\,o})_{SO_2} \quad \text{(A-20)}$$

So computing the value of $h_{R2}(1kmol) = 685537.87$ kJ/kmol

Since we assume the full conversion of SO_2 above is the final heat of reaction.

So overall heat of reaction is given by the following equation:

$$h_R = h_{R1} + h_{R2} = -482447.08 + 685537.87 = 170962.70 \text{ kJ/kmol}$$

Above is the calculated heat of the reaction.

Simulated heat of reaction is:

$$h_R = h_{R1} + h_{R2} = -518023.99 + 685981.99 = 167958.00 \text{ kJ/kmol}$$

We can observe that the observed and calculated heats of reactions are nearly equal. This verifies the energy balance of the Claus Furnace.

Fig. A-15 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

RStoic results

Outlet temperature:	2011.99999	F
Outlet pressure:	24.7	psi
Heat duty:	0.02207234	MW
Net heat duty:	0.02207234	MW
Vapor fraction:	1	
1st liquid / Total liquid:		

Mass and energy balance

Total		In	Out	Generated	Rel. diff
Mole-flow:	lbmol/hr	14.5555303	15.4856688	0.93013844	1.4339E-17
Mass-flow:	lb/hr	476.091526	476.091526		1.194E-16
Enthalpy:	MW	-0.0193407	0.00273163		-1.1412374

Fig. A-15 Mass and energy balance results around Claus furnace

Energy Balance around COOLER5:
Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the table A-16

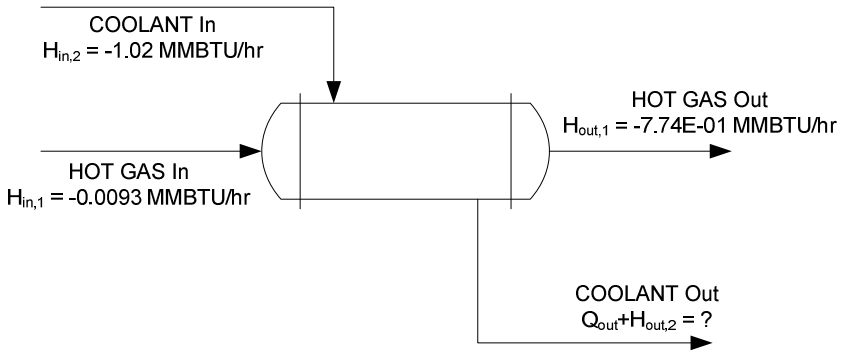


Fig. A-16 Energy balance around cooler5

In the cooler no heat is supplied in, so Q_{in} = 0 MMBTU/hr

Similarly since no work is done in a cooler $W_{in} = W_{out} = 0$ MMBTU/hr

Overall Energy balance around the Cooler is given by Eqs. A-11, A12, A-13, and A-14:

So $H_{2,out}+Q_{out}$ = -0.0093 – 1.02 + 7.74E-01 + 2.39E-01
= 5.0741E-05 MMBTU/hr

So above is the heat duty of the cooler. The heat rejected is accompanied with steam. Fig. A-17 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

Heatx results

	Inlet		Outlet	
Hot stream:	CLAUS1		CLAUS2	
Temperature:	2011.99999	F	250	F
Pressure:	24.7	psi	24.7	psi
Vapor fraction:	1		0.75272699	
Cold stream:	COOLWTR4		H2OST4	
Temperature:	77	F	1432.41116	F
Pressure:	14.7	psi	14.7	psi
Vapor fraction:	0		1	
Heat duty:	0.07552903	MW		

Mass and energy balance

Total		In	Out	Rel. diff
Mole-flow:	lbmol/hr	23.811934	23.811934	0
Mass-flow:	lb/hr	626.091526	626.091526	0
Enthalpy:	MW	-0.2969765	-0.2969766	1.0151E-07

Fig. A-17 Mass and energy balance results around cooler5

Energy Balance around CLAUSSEP:
Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the Fig. A-18.

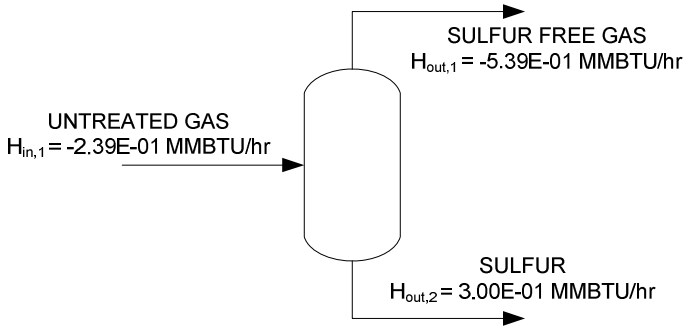


Fig. A-18 Energy balance around Claus separator

From the energy balance equation we can determine the work done by the separator:

$$W_{out} = \Sigma H_{in} - \Sigma H_{out} + Q_{in} - Q_{out} \qquad \text{(A-21)}$$

Since there is no heat transfer in the separator $Q_{in} = Q_{out} = 0$

So the work done by the separator is given as $W_{out} = -2.39E-01 + 5.39E-01 - 3.00E-01$

$$= -9.00E-06 \text{MMBTU/hr}$$

Above work done is the heat duty of the separator.

Simulated heat duty from Aspen is found to be -8.98E-06 MMBTU/hr

Separation Efficiency:

Amount of sulfur entering the Separator = 94.45 lb/hr

Amount of sulfur removed = 94.40 lb/hr

Calculated % Recovery = 99.94

Fig. A-19 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

Block results summary

Outlet temperature:	249.999929	F
Outlet pressure:	24.7	psi
Vapor fraction:	0.75272691	
Heat duty:	0	MW
Net duty:	0	MW

Mass and energy balance

Total		In	Out	Rel. diff
Mole-flow:	lbmol/hr	15.4856688	15.4856688	0
Mass-flow:	lb/hr	476.091526	476.091526	0
Enthalpy:	MW	-0.0727974	-0.0727974	5.8837E-08

Fig. A-19 Mass and energy balance results around Claus separator

Energy Balance around CLAUSHR2:
Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the table A-20.

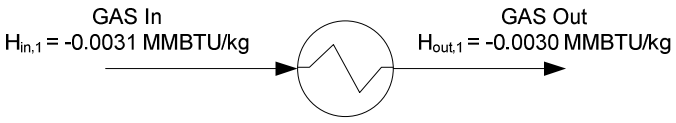


Fig. A-20 Energy balance around Claus heat exchanger

In the cooler no heat is supplied in, so Q_{in} = 0 MMBTU/hr

Similarly since no work is done in a cooler $W_{in} = W_{out}$ = 0 MMBTU/hr

Overall Energy balance around the Cooler is given by Eqs. A-11, A12, and A-13:

Mass of Stream entering and leaving = $\dot{m}$ = 375.29 lb/hr = 170.23 kg/hr

So Q_{out} = mass of stream $\times (H_{in} \; H_{out})$

= -0.024 MMBTU/hr

So above is the heat duty of the cooler. The heat rejected is accompanied with steam.

Fig. A-21 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

Block results summary

Outlet temperature:	495.5	F
Outlet pressure:	24.7	psi
Vapor fraction:	1	
Heat duty:	0.00677991	MW
Net duty:	0.00677991	MW
1st liquid / Total liquid:		
Pressure-drop correlation parameter:	0	

Mass and energy balance

Total		In	Out	Rel. diff
Mole-flow:	lbmol/hr	11.6564795	11.6564795	0
Mass-flow:	lb/hr	364.971913	364.971913	-1.557E-16
Enthalpy:	MW	-0.1417496	-0.1349697	-0.0478302

Fig. A-21 Mass and energy balance results around Claus heat exchanger

Energy Balance around Claus Furnace (CFURNACE2):
Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the table A-22.

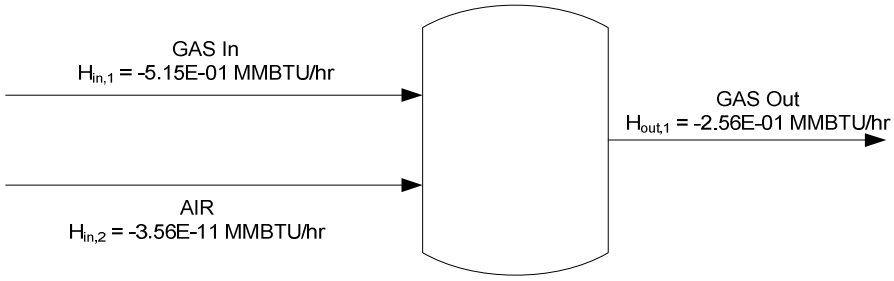


Fig. A-22 Energy balance around Claus furnace

So the overall heat duty of the furnace is given by

$$Q_{in} = \Sigma H_{out} - \sum H_{in} \qquad \text{(A-22)}$$

So Heat duty of the furnace is Q_{in} = -2.56E-01 + 5.15E-01 + 3.56E-11
= 0.26 MMBTU/hr (Calculated)

Simulated heat duty of the furnace = 0.2584 MMBTU/hr

Fig. A-23 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

RStoic results

Outlet temperature:	1201.99999	F
Outlet pressure:	24.7	psi
Heat duty:	254491.364	Btu/hr
Net heat duty:	254491.364	Btu/hr

Mass and energy balance

Total		In	Out	Generated	Rel. diff
Mole-flow:	lbmol/hr	13.1564795	14.2882159	1.13173636	-6.216E-17
Mass-flow:	lb/hr	412.631102	412.631102		1.3776E-16
Enthalpy:	MW	-0.1349697	-0.0603856		-0.5525987

Fig. A-23 Mass and energy balance results around Claus furnace

Energy balance around CLAUSSP2:
Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the Fig. A-24.

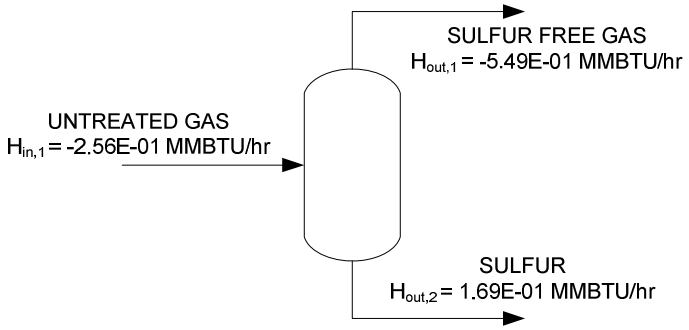


Fig. A-24 Energy balance around Claus separator

From the energy balance equation we can determine the work done by the separator:

$$W_{out} = \Sigma H_{in} - \Sigma H_{out} + Q_{in} - Q_{out} \qquad \text{(A-23)}$$

Since there is no heat transfer in the separator $Q_{in} = Q_{out} = 0$

So the work done by the separator is given as $W_{out} = -2.56E-01 + 5.49E-01 - 1.690E-01$

$$= 1.25E-01 \text{MMBTU/hr}$$

Above work done is the heat duty of the separator.

Simulated heat duty from Aspen is found to be 1.2457E-01 MMBTU/hr

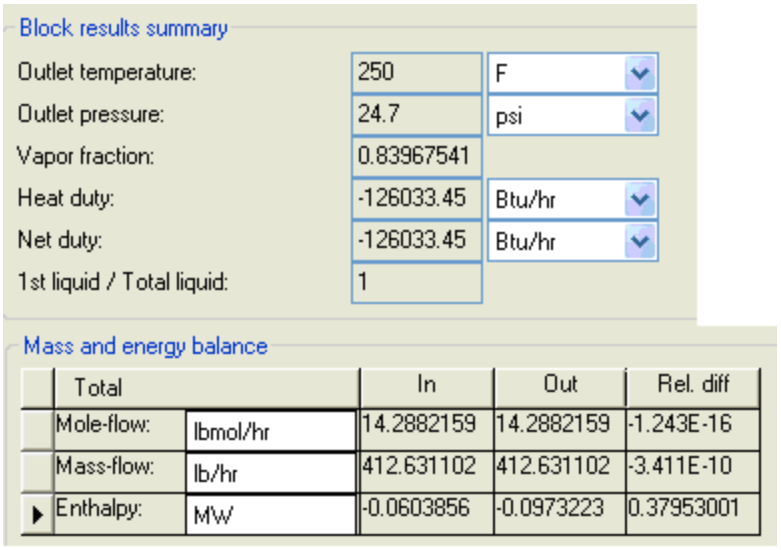
Separation Efficiency:

Amount of sulfur entering the Separator = 1.704 lb/hr

Amount of sulfur removed = 1.702 lb/hr

Calculated % Recovery = 99.89

Fig. A-25 shows the results of the unit operation pump with Mass and energy balance around the unit operation.



Block results summary

Outlet temperature:	250	F
Outlet pressure:	24.7	psi
Vapor fraction:	0.83967541	
Heat duty:	-126033.45	Btu/hr
Net duty:	-126033.45	Btu/hr
1st liquid / Total liquid:	1	

Mass and energy balance

Total		In	Out	Rel. diff
Mole-flow:	lbmol/hr	14.2882159	14.2882159	-1.243E-16
Mass-flow:	lb/hr	412.631102	412.631102	-3.411E-10
Enthalpy:	MW	-0.0603856	-0.0973223	0.37953001

Fig. A-25 Mass and energy balance results around Claus separator

Gas Turbine

Energy Balance around GTCOMP2:

Compressor is used to compress the cleaned and cooled syngas for the gas turbine section to certain higher pressure. This is the first stage of two stage compression process.

Inlet Pressure of Oxygen Stream Entering Compressor = 50 psia

Outlet Pressure of Oxygen coming out of Compressor = 150 psia

Compression Ratio value from Aspen $\gamma = 1.3926$

Inlet Temperature of Oxygen Stream = 428.58 K

Molecular weight of the syngas stream from Aspen= 28.65 kg/kmol

So R in terms of (kJ/kg K) is given as = $\dfrac{\text{R (in kJ/kmol K)}}{\text{Molecular Weight}}$

$$= \frac{8.314}{28.6524} = 0.2901 \text{ kJ/kg K}$$

Work done by the Compressor (W_{in}) is given by the following equation.

$$W_{comp,\,in} = \frac{\gamma R T_{in}}{\gamma - 1}\left(\left(\frac{P_{out}}{P_{in}}\right)^{\left(\frac{\gamma-1}{\gamma}\right)} - 1\right) \qquad \text{(A-24)}$$

Using the above equation calculating the value of $W_{comp,in} =$ 160.15 kJ/kg

Mass of syngas entered into the compressor = ($\dot{m}$) = 15489.74 kg/hr

$$\text{So amount of } W_{comp,\,in} \text{ in kJ/hr} = \text{Mass of syngas Entered} \times \text{Work (in kJ/kg)}$$

$$= 160.15 \times 15489.74 = 2480697.46 \text{ kJ/hr}$$

$$= 2351247.47 \text{ BTU/hr}$$

But the above calculated work done is for 100% efficient compressor. So Work input for a 92% isentropic efficient compressor is given by:

$$\frac{\text{Work done at 100\% efficiency}}{\text{Isentropic Efficiency}} \qquad \text{(A-25)}$$

$$\text{So final work input for the compressor is} = \frac{2351247.47}{0.92} = 2555703.77 \text{ BTU/hr}$$

The mechanical efficiency of the compressor was assumed to be 98%. So final work done with 98% mechanical efficiency is given as:

$$= \frac{2.5557}{0.98} = 2.61 \text{ MMBTU/hr}$$

Overall Enthalpy balance around compressor is given as:

Energy In = Energy Out

which is given by the following equations:

$$E_{in} = W_{in} + \dot{m}H_1 + \left(\frac{\dot{m}v^2}{2}\right) + \dot{m}gz_1 \qquad \text{(A-26)}$$

$$E_{out} = Q_{out} + \dot{m}H_2 + \left(\frac{\dot{m}v^2}{2}\right) + \dot{m}gz_2 \qquad \text{(A-27)}$$

Neglecting the potential and kinetic energy effects we can calculate the final heat out from the compressor (Q_{out})

Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the Fig. A-26.

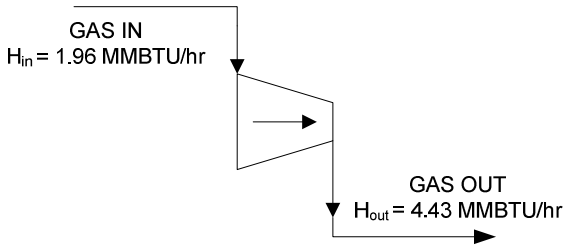


Fig. A-26 Energy balance of the first gas turbine compressor

So from the Balance $Q_{out} = W_{comp,in} + H_{in} - H_{out}$

So Q_{out} = 2.6078 +1.96E-00 – 4.43E-00 = 1.36E-01 MMBTU/hr

Cross Check:

Enthalpy of Inlet stream (COMPGA1) H_{in} = 1.96E+00 MMBTU/hr

Enthalpy of outlet stream (COMPGA2) H_{out} = 4.43E+00 MMBTU/hr

By energy balance $H_{in} - H_{out} = Q_{out} - W_{comp,in}$

= 1.96E+00 – 4.43E+00 = -2.47E+00 MMBTU/hr

From Calculated values of $Q_{out} - W_{comp,in}$ = 1.36E-01 – 2.6078 = -2.47E+00 MMBTU/hr

Fig. A-27 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

Compr results

Compressor model:	Isentropic Compressor	
Phase calculations:	Vapor phase calculation	
Indicated horsepower:	0.57380876	MW
Brake horsepower:	0.60400922	MW
Net work required:	0.60400922	MW
Power loss:	0.03020046	MW
Efficiency:	0.95	
Mechanical efficiency:	0.95	
Outlet pressure:	50	psi
Outlet temperature:	311.788095	F
Isentropic outlet temperature:	300.120945	F
Vapor fraction:	1	
Displacement:		
Volumetric efficiency:		

Fig. A-27 Mass and energy balance results of the first gas turbine compressor

Energy Balance around GTCOMP3:

Compressor is used to compress the cleaned and cooled syngas for the gas turbine section to certain higher pressure. This is the second of two stage compression process. Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the Fig. A-28.

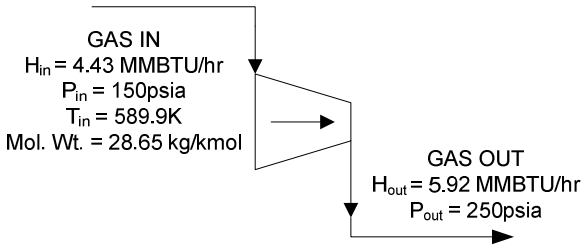


Fig. A-28 Energy balance around second gas turbine compressor

Compression Ratio value from Aspen $\gamma = 1.3771$

So R in terms of (kJ/kg K) is given as = R (in kJ/kmol K) / Molecular Weight

= 8.314 / 28.65 = 0.29 kJ/kg K

Work done by the compressor (Win) is given by Eq. A-24.

Using the above equation calculating the value of $W_{comp,in}$ = 93.86 kJ/kg

Mass of syngas entered into the compressor = ($\dot{m}$) = 15489.74 kg/hr

$$\text{So amount of } W_{comp,in} \text{ in kJ/hr} = \text{Mass of syngas Entered} \times \text{Work (in kJ/kg)}$$
$$= 93.86 \times 15489.74 = 1453931.70 \text{ kJ/hr}$$

= 1378061.33 BTU/hr

But the above calculated work done is for 100% efficient compressor. So Work input for a 92% isentropic efficient compressor is given by:

$$\frac{\text{Work done at 100\% efficiency}}{\text{Isentropic Efficiency}}$$

$$\text{So final work input for the compressor is} = \frac{1378061.33}{0.92} = 1497892.75 \text{ BTU/hr}$$
= 1.49 MMBTU/hr

The mechanical efficiency of the compressor was assumed to be 100%. So final work done with 100% mechanical efficiency is given as:

$$= \frac{1.4978}{1.00} = 1.49 \text{ MMBTU/hr}$$

Overall Enthalpy balance around compressor is given as:

Energy In = Energy Out

which is given by the following Eqs. A-26 and A-27:

Neglecting the potential and kinetic energy effects we can calculate the final heat out from the compressor (Q_{out})

So from the Balance $Q_{out} = W_{comp,in} + H_{in} - H_{out}$

So Q_{out} = 1.49 +4.43E-00 – 5.92E-00 = 6.03E-04 MMBTU/hr

Cross Check:

Enthalpy of Inlet stream (COMPGA2) H_{in} from Aspen = 4.4299E+00 MMBTU/hr

Enthalpy of outlet stream (COMPGA3) H_{out} from Aspen = 5.9272E+00 MMBTU/hr

By energy balance $H_{in} - H_{out} = Q_{out} - W_{comp,in}$

$= 4.4299E+00 - 5.9272E+00 = -1.497E+00$ MMBTU/hr

From Calculated values of $Q_{out} - W_{comp,in} = 6.03E-04 - 1.4978 = -1.497E+00$ MMBTU/hr

Fig. A-29 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

Compr results

Compressor model:	Isentropic Compressor	
Phase calculations:	Vapor phase calculation	
Indicated horsepower:	0.72447388	MW
Brake horsepower:	0.76260408	MW
Net work required:	0.76260408	MW
Power loss:	0.03813020	MW
Efficiency:	0.95	
Mechanical efficiency:	0.95	
Outlet pressure:	150	psi
Outlet temperature:	602.320278	F
Isentropic outlet temperature:	588.006671	F
Vapor fraction:	1	
Displacement:		
Volumetric efficiency:		

Fig. A-29 Mass and energy balance results of the second gas turbine compressor

Energy Balance around Gas Turbine 1: (GTTURB1)
Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the Fig. A-30.

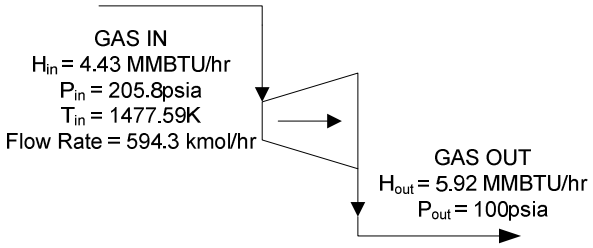


Fig. A-30 Energy balance around first gas turbine

Compression Ratio value from Aspen γ = 1.277

So we know that $\frac{c_P}{c_V} = \gamma$ (A-28)

We also know that $c_P - c_V = R$ (A-29)

The value of R = 8.314 kJ/kmol K

So $c_V = \frac{R}{\gamma - 1}$ = 30.0065 kJ/kmol K

Hence c_P = 38.3205 kJ/kmol K

Turbine Pressure Ratio (TPR) is given by:

$$TPR = \frac{P_{out}}{P_{in}} = \left(\frac{T_{out}}{T_{in}}\right)^{\frac{\gamma}{\gamma-1}} \quad \text{(A-30)}$$

Turbine pressure ratio is then calculated as = 100 / 205.8 = 0.4859

Now we can calculate the turbine work. Turbine work is computed as:

$$TurbineWork = \eta_{It} c_p T_{in} \left(1 - TPR^{(\gamma-1)/\gamma}\right) \quad \text{(A-31)}$$

Where: Isentropic Efficiency η_{It} of the turbine is assumed to be 95%

Now calculating the work done by the turbine:

$= (0.95 \times 38.3205 \times 1477.594) \times (1 - (0.4859^{((1.277-1)/1.277)})) =$ 7796.64 kJ/kmol

Molar flow rate of the syngas in the turbine = 594.315 kmol/hr

$$= 4.3918 \text{ MMBTU/hr}$$

So work done by the turbine $= 7796.64 \times 594.315 = 4633666.346$ kJ/hr

Now with mechanical efficiency of 95% for the turbine we have:

Net work available to the shaft from the turbine is : $4.3918 \times 0.95 = 4.17$ MMBTU/hr

Simulated value of available shaft work from Aspen = 4.17 MMBTU/hr

So from the energy balance heat released during the expansion process (Q_{out}) is given as

$$Q_{out} = \Sigma H_{in} - \sum H_{out} - W_{out} \qquad \text{(A-32)}$$

So Calculating the value of Q_{out} = -1.06+E01 + 1.50E+01 + 4.17

$$= 0.217 \text{ MMBTU/hr}$$

Fig. A-31 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

Compr results

Compressor model:	Isentropic Turbine	
Phase calculations:	Vapor phase calculation	
Indicated horsepower:	-1.2863985	MW
Brake horsepower:	-1.2220785	MW
Net work required:	-1.2220785	MW
Power loss:	0.06431992	MW
Efficiency:	0.95	
Mechanical efficiency:	0.95	
Outlet pressure:	100	psi
Outlet temperature:	1829.85213	F
Isentropic outlet temperature:	1810.11185	F
Vapor fraction:	1	
Displacement:		
Volumetric efficiency:		

Fig. A-31 Mass and energy balance results around the first gas turbine

Energy Balance around Gas Turbine 2: (GTTURB2)
Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the Fig. A-32.

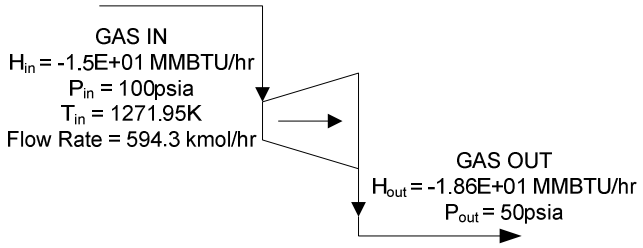


Fig. A-32 Energy balance around second gas turbine

Compression Ratio value from Aspen $\gamma = 1.2856$

So we know that $\frac{c_P}{c_V} = \gamma$

We also know that $c_P - c_V = R$

The value of R = 8.314 kJ/kmol K

So $c_V = \frac{R}{\gamma - 1} = 29.1080$ kJ/kmol K

Hence c_P = 37.4220 kJ/kmol K

Turbine Pressure Ratio (TPR) is given by Eq. A-30

Pressure of inlet stream (p_{in}) = 100 psia

Pressure of outlet stream coming out of turbine (p_{out}) = 50 psia

Turbine pressure ratio is then calculated as = 50/100 = 0.5

Now we can calculate the turbine work. Turbine work is computed using A-31:

Where:

Isentropic Efficiency η_{I_t} of the turbine is assumed to be 95%

Now calculating the work done by the turbine:

$$= (0.95 \times 37.4220 \times 1271.95) \times (1 - (0.5^{((1.2856-1)/1.2856))}) = \quad 6453.88 \text{ kJ/kmol}$$

Molar flow rate of the syngas in the turbine = 594.315 kmol/hr

So work done by the turbine = $6453.88 \times 594.315 = 3835643.104$ kJ/hr

$$= 3.6354 \text{ MMBTU/hr}$$

Now with mechanical efficiency of 95% for the turbine we have:

Net work available to the shaft from the turbine is : $3.6354 \times 0.95 = 3.4537$ MMBTU/hr
Simulated value of available shaft work from Aspen = 3.4515 MMBTU/hr
So from the energy balance heat released during the expansion process (Q_{out}) is given by Eq. A-32

So Calculating the value of Q_{out} = -1.50+E01 + 1.86E+01 + 3.4537

$$= 0.179 \text{ MMBTU/hr}$$

Fig. A-33 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

Compr results

Compressor model:	Isentropic Turbine	
Phase calculations:	Vapor phase calculation	
Indicated horsepower:	-1.0647825	MW
Brake horsepower:	-1.0115434	MW
Net work required:	-1.0115434	MW
Power loss:	0.05323912	MW
Efficiency:	0.95	
Mechanical efficiency:	0.95	
Outlet pressure:	50	psi
Outlet temperature:	1515.69098	F
Isentropic outlet temperature:	1498.91371	F
Vapor fraction:	1	
Displacement:		
Volumetric efficiency:		

Fig. A-33 Mass and energy balance results around the second gas turbine

Energy Balance around Gas Turbine 3: (GTTURB3)
Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the Fig. A-34.

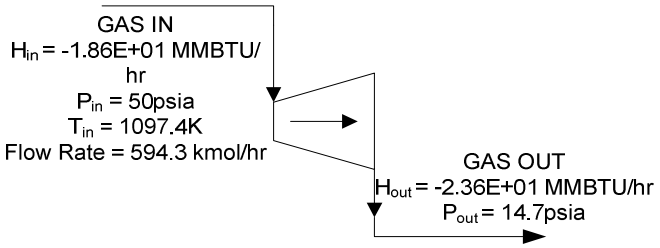


Fig. A-34 Energy balance around third gas turbine

Compression Ratio value from Aspen γ = 1.2955

So we know that $\frac{c_P}{c_V} = \gamma$

We also know that $c_P - c_V = R$

The value of R = 8.314 kJ/kmol K

So $c_V = \frac{R}{\gamma - 1}$ = 28.1339 kJ/kmol K

Hence cP = 36.4479 kJ/kmol Ks

Turbine Pressure Ratio (TPR) is given by Eq. A-30

Turbine pressure ratio is then calculated as = 14.7/50 = 0.294

Now we can calculate the turbine work. Turbine work is computed using Eq. A-31

Where:

Isentropic Efficiency η_{It} of the turbine is assumed to be 95%

Temperature of the inlet stream = 1097.42 K

Now calculating the work done by the turbine:

$$= (0.95 \times 36.45 \times 1097.42) \times (1 - (0.294^{((1.2955-1)/1.2955))}) = \quad 8965.80 \text{ kJ/kmol}$$

Molar flow rate of the syngas in the turbine = 594.32 kmol/hr

So work done by the turbine $= 8965.8006 \times 594.315 = 5328517.198$ kJ/hr

= 5.05 MMBTU/hr

Now with mechanical efficiency of 90% for the turbine we have:

Net work available to the shaft from the turbine is : $5.05 \times 0.90 = 4.54$ MMBTU/hr

Simulated value of available shaft work from Aspen = 4.53 MMBTU/hr

So from the energy balance heat released during the expansion process (Q_{out}) is given by Eq. A-32

So Calculating the value of Q_{out} = -1.86+E01 + 2.36E+01 + 4.5347

= 0.494 MMBTU/hr

Fig. A-35 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

Compr results

Compressor model:	Isentropic Turbine	
Phase calculations:	Vapor phase calculation	
Indicated horsepower:	-1.4766725	MW
Brake horsepower:	-1.3290052	MW
Net work required:	-1.3290052	MW
Power loss:	0.14766725	MW
Efficiency:	0.92	
Mechanical efficiency:	0.9	
Outlet pressure:	14.7	psi
Outlet temperature:	1063.27715	F
Isentropic outlet temperature:	1022.76282	F
Vapor fraction:	1	
Displacement:		
Volumetric efficiency:		

Fig. A-35 Mass and energy balance results around the third gas turbine

Steam Turbine and HRSG

Energy Balance around HRSG1:

Heat Recover Steam Generator (HRSG) acts as a coupling point to collect different steam streams. The steams generated in various sections are routed to this coupling point where it's reheated and pressurized and sent into the steam turbine.

The energy balance equations used in the HRSG section are:

$$E_{in} = Q_{win+} \dot{m}_w (h_{w,in}) \quad \text{(A-33)}$$

$$E_{out} = \dot{m}_w (h_{w,out}) \quad \text{(A-34)}$$

$$Q_{win} = \dot{m}_w (h_{w,out} - h_{w,in}) \quad \text{(A-35)}$$

HRSG1 is used to generate steam from high temperature gas which comes out of the gas turbine section.

Energy temperature from hot gas to the cooling water is found using the above equations.

Enthalpy of the Water in (HRSGWTR1) @ 77 F = -6817.64 BTU/lb

= -15857.84 BTU/kg

Enthalpy of the Water Out (H2OST5) @ 1056.77 F = -5431.99 BTU/lb

= -12634.80 BTU/kg

Mass of water entering the heat exchanger (m) = 1088.62 kg/hr

Now calculating Q_{win} from the following equation:

$$Q_{win} = \dot{m}_w (h_{w,out} - h_{w,in}) \quad \text{(A-36)}$$

$$= 1088.62 \times (-12634.80 + 15857.84) = 3508664.69 \text{ BTU/hr}$$

= 3.51 MMBTU/hr

With 95% heat efficiency transfer we have:

$$= 3.51 \times 0.95 = 3.33 \text{ MMBTU/hr}$$

Heat duty value from Aspen simulation is = 3.3255 MMBTU/hr

Fig. A-36 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

Heatx results

	Inlet		Outlet	
Hot stream:	HRGAS1		WASTEGAS	
Temperature:	1063.27715	F	750	F
Pressure:	14.7	psi	14.7	psi
Vapor fraction:	1		1	
Cold stream:	HRSGWTR1		H2OST5	
Temperature:	77	F	800.482607	F
Pressure:	14.7	psi	14.7	psi
Vapor fraction:	0		1	
Heat duty:	0.97462915	MW		

Mass and energy balance

Total		In	Out	Rel. diff
Mole-flow:	lbmol/hr	1443.46182	1443.46182	0
Mass-flow:	lb/hr	41038.3598	41038.3598	0
Enthalpy:	MW	-11.724144	-11.724144	-1.007E-08

Fig. A-36 Mass and energy balance results around the first HRSG

Energy Balance around HRSG2:

Heat Recover Steam Generator (HRSG) acts as a coupling point to collect different steam streams. The steams generated in various sections are routed to this coupling point where it's reheated and pressurized and sent into the steam turbine.

The energy balance equations used in the HRSG section are given by Eqs. A-33, A-34, and A-35.

HRSG2 is the second stage used to generate steam from high temperature gas which comes out of the gas turbine section.
Energy temperature from hot gas to the cooling water is found using the above equations.
Enthalpy of the Water in (HRSGWTR2) @ 77 F = -6.82E+03 BTU/lb

= -15857.84 BTU/kg

Enthalpy of the Water Out (H2OST6) @ 1056.77 F = -5.47E+03 BTU/lb

= -12715.55 BTU/kg

Mass of water entering the heat exchanger (m) = 687.19 kg/hr

Now calculating Q_{win} using Eq. A-36:

$$= 687.19 \times (-12715.55 + 15857.84) = 2159352.59 \text{ BTU/hr}$$

= 2.16 MMBTU/hr

With 95% heat efficiency transfer we have:

$$= 2.16 \times 0.95 = 2.05 \text{ MMBTU/hr}$$

Heat duty value from Aspen simulation is = 2.0466 MMBTU/hr

Fig. A-37 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

Heatx results

	Inlet		Outlet	
Hot stream:	WASTEGAS		WASTEGA1	
Temperature:	750	F	550	F
Pressure:	14.7	psi	14.7	psi
Vapor fraction:	1		1	
Cold stream:	HRSGWTR2		H2OST6	
Temperature:	77	F	730.228513	F
Pressure:	14.7	psi	14.7	psi
Vapor fraction:	0		1	
Heat duty:	0.59982026	MW		

Mass and energy balance

Total		In	Out	Rel. diff
Mole-flow:	lbmol/hr	1394.33685	1394.33685	0
Mass-flow:	lb/hr	40153.3598	40153.3598	0
Enthalpy:	MW	-10.930495	-10.930495	6.0403E-09

Fig. A-37 Mass and energy balance results around the second HRSG

Energy Balance around Reboiler:

Heat duty of the reboiler is given by the equation:

$$Q_{win} = \dot{m}_w (h_{products} - h_{reactants}) \qquad \text{(A-37)}$$

Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the table A-38.

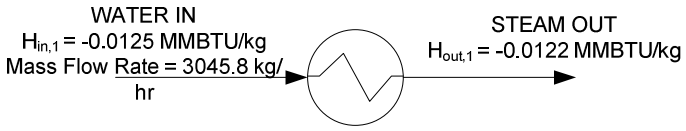


Fig. A-38 Energy balance around re-boiler

$$\text{Heat duty of the reboiler} = 3045.87 \times (-12264.38 + 12583.83)$$

$$= 973005.7561 \text{ BTU/hr} = 0.9730 \text{ MMBTU/hr}$$

Aspen simulated value of the heat duty of the reboiler = 0.9522 MMBTU/hr

Fig. A-39 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

Block results summary

Outlet temperature:	1112	F
Outlet pressure:	2175.75	psi
Vapor fraction:	1	
Heat duty:	0.26761219	MW
Net duty:	0.26761219	MW
1st liquid / Total liquid:		
Pressure-drop correlation parameter:	-12491265	

Mass and energy balance

Total		In	Out	Rel. diff
Mole-flow:	lbmol/hr	372.739141	372.739141	0
Mass-flow:	lb/hr	6715	6715	0
Enthalpy:	MW	-10.644206	-10.376594	-0.0251415

Fig. A-38 Mass and energy balance results around re-boiler

Energy balance around HP turbine:

High-pressure turbine forms the first stage of the two stage turbine in the steam cycle process. Rankine cycle was used to model the steam cycle process.

The shaft work available in the turbine can be estimated using the following equations:

$$E_{in} = W_{in} + Q_{in} + \dot{m}\ (h_{in}) \qquad \text{(A-38)}$$

$$E_{out} = W_{out} + Q_{out} + \dot{m}(h_{out}) \qquad \text{(A-39)}$$

In a heat in and heat out are assumed to be zero. Even though there is slight heat dissipation due to the shaft work it can be considered as negligible.

Hence $Q_{in} = Q_{out} =$ 0 MMBTU/hr

Similarly work in is also considered to be zero = W_{in} = 0 MMBTU/hr

So Work available for the shaft work is given as

$$W_{out} = dH + d(KE) + d(PE) \qquad \text{(A-40)}$$

Neglecting the kinetic and potential energy changes as they are infinitesimal, we have:

$$W_{out} = dH \qquad \text{(A-41)}$$

So enthalpy of the inlet and outlet streams from aspen in the Fig. A-40:

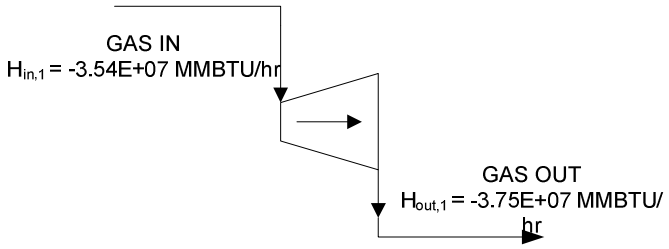


Fig. A-40 Energy balance around high-pressure steam turbine

So shaft work available due to expansion = W_{out} = -3.54E+07 + 3.75E+07

= 2.077 MMBTU/hr

With 95% efficiency of the turbine the ultimate shaft power available =

$= 2.077 \times 0.95 = 1.97315$ MMBTU/hr

= 0.5782 MW

Simulated value of the W_{out} = 1.9726 MMBTU/hr

Fig. A-41 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

Compr results

Compressor model:	Isentropic Turbine	
Phase calculations:	Two phase calculation	
Indicated horsepower:	-0.6085481	MW
Brake horsepower:	-0.5781207	MW
Net work required:	-0.5781207	MW
Power loss:	0.03042740	MW
Efficiency:	0.92	
Mechanical efficiency:	0.95	
Outlet pressure:	174.045285	psi
Outlet temperature:	490.595653	F
Isentropic outlet temperature:	433.231937	F
Vapor fraction:	1	
Displacement:		
Volumetric efficiency:		

Fig. A-41 Mass and energy balance results around high pressure steam turbine

Energy balance around LP turbine:
Low-pressure turbine forms the second stage of the two stage turbine in the steam cycle process. Rankine cycle was used to model the steam cycle process.
The shaft work available in the turbine can be estimated using Eqs. A-38 and A-39:

In a heat in and heat out are assumed to be zero. Even though there is slight heat dissipation due to the shaft work it can be considered as negligible.

Hence $Q_{in} = Q_{out} =$ 0 MMBTU/hr

Similarly work in is also considered to be zero = $W_{in} = 0$ MMBTU/hr

So Work available for the shaft work is given by Eq. A-40

Neglecting the kinetic and potential energy changes as they are infinitesimal, we have Eq. A-41.

So enthalpy of the inlet and outlet streams from aspen is given as:

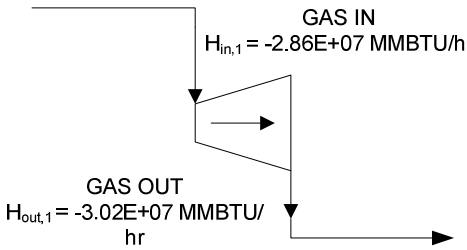


Fig. A-42 Energy balance around low pressure steam turbine

So shaft work available due to expansion = W_{out} = -2.86E+07 + 3.02E+07

= 1.617 MMBTU/hr

With 95% efficiency of the turbine the ultimate shaft power available =

$= 1.617 \times 0.95 = 1.5361$ MMBTU/hr

= 0.4502 MW

Simulated value of the W_{out} = 1.5363 MMBTU/hr

Fig. A-43 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

Compr results

Compressor model:	Isentropic Turbine	
Phase calculations:	Two phase calculation	
Indicated horsepower:	-0.2820242	MW
Brake horsepower:	-0.267923	MW
Net work required:	-0.267923	MW
Power loss:	0.01410121	MW
Efficiency:	0.92	
Mechanical efficiency:	0.95	
Outlet pressure:	14.7	psi
Outlet temperature:	212.046026	F
Isentropic outlet temperature:	212.046026	F
Vapor fraction:	0.93890271	
Displacement:		
Volumetric efficiency:		

Fig. A-43 Mass and energy balance results around low pressure steam turbine

Energy Balance around Condenser:

Heat duty of the condenser is given by the equation:

$$Q_{win} = \dot{m}_w (h_{products} - h_{reactants}) \qquad \text{(A-42)}$$

Main parameters of inlet and outlet stream associated with the unit operation process which is used in the calculation are shown in the Fig. A-44.

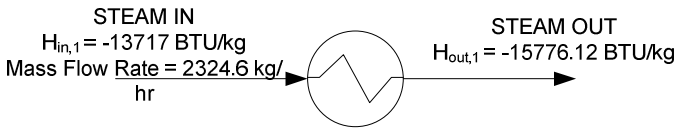


Fig. A-44 Energy balance around condenser

$$\text{Heat duty of the reboiler} = 2324.610 \times (-15776.12\ 6 + 13717.649)$$

Aspen simulated value of the heat duty of the reboiler = -4.6354569 MMBTU/hr

Table A-4 shows a comparison between the computed energy balance values with that of simulated ones for various unit operations in gasification island, cooling section and claus process.

Fig. A-45 shows the results of the unit operation pump with Mass and energy balance around the unit operation.

Block results summary

Outlet temperature:	212.045821	F
Outlet pressure:	14.7	psi
Vapor fraction:	0	
Heat duty:	-1.3729868	MW
Net duty:	-1.3729868	MW
1st liquid / Total liquid:	1	
Pressure-drop correlation parameter:	0	

Mass and energy balance

Total		In	Out	Rel. diff
Mole-flow:	lbmol/hr	284.474513	284.474513	0
Mass-flow:	lb/hr	5124.888	5124.888	0
Enthalpy:	MW	-8.6658846	-10.038871	0.13676705

Fig. A-45 Mass and energy balance results around condenser

Table A-4 Energy balance comparison in gas cooling and Claus process

Unit Operation	Property (units)	This Work	Aspen	Difference
Gasification Section				
Pump	Work Done (MMBTU/hr)	0.0009	0.0009	+0.000
Compressor	Work Done (MMBTU/hr)	0.440	0.4404	-0.0004
Gasifier	Heat Duty (MMBTU/hr)	0.9284	0.9285	-0.0001
Cooling Section				
Cooler 1	Heat Out (MMBTU/hr)	3.919	3.920	+0.001
Cooler 2	Heat Out (MMBTU/hr)	4.605	4.600	-0.005
Cooler 3	Heat Out (MMBTU/hr)	5.712	5.710	-0.002
Claus Process				
Claus Furnace	Heat of reaction (kJ/kmol)	1.709×10^{5}	1.679×10^{5}	-0.03×10^{5}
Claus Cooler	Heat Out (MMBTU/hr)	0.00	5.04×10^{-5}	-5.04×10^{-5}
Claus Separator	Work Out (MMBTU/hr)	0.00	9×10^{-6}	-9×10^{-6}
Claus Heat Exchanger	Heat Duty (MMBTU/hr)	0.0245	0.0245	0.000
Claus Furnace 2	Heat Duty (MMBTU/hr)	0.2585	0.25849	-0.00001
Claus Separator	Heat Duty (MMBTU/hr)	0.12457	0.12457	0.000

Table A-5 shows the a comparison between the computed energy balance values with that of simulated ones for various unit operations in gas turbine section and steam turbine section.

Table A-5 Energy balance comparison in gas and steam turbine section

Unit Operation	Property (units)	This Work	Aspen	Difference
Gas Turbine Section				
Compressor 1	$Work_{In} + Q_{out}$ (MMBTU/hr)	2.472	2.4719	-0.0001
Compressor 2	$Work_{In} + Q_{out}$ (MMBTU/hr)	1.497	1.497	0.000
Gas Turbine 1	Shaft Work (MMBTU/hr)	4.1722	4.1699	-0.0023
Gas Turbine 2	Shaft Work (MMBTU/hr)	3.4537	3.4515	-0.0022
Gas Turbine 3	Shaft Work (MMBTU/hr)	4.5454	4.5347	-0.0107
HRSG and Steam Cycle				
HRSG Heat Exchanger 1	Heat Duty (MMBTU/hr)	3.3332	3.3255	-0.0076
HRSG Heat Exchanger 2	Heat Duty (MMBTU/hr)	2.0513	2.0466	-0.0047
Reboiler	Heat Duty (MMBTU/hr)	0.9730	0.9522	-0.0207
High-pressure Steam Turbine	Shaft Work (MMBTU/hr)	1.9731	1.9726	-0.0005
Low-pressure Steam Turbine	Shaft Work (MMBTU/hr)	1.5361	1.5363	-0.0002
Condenser	Heat Duty (MMBTU/hr)	4.7851	4.6354	0.1497

VITA

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